Lecture Notes on Hilbert Spaces and Quantum Mechanics

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I.1 Introduction

The concept of a Hilbert space is seemingly technical and special. For example, the reader has probably heard of the space ℓ^2 (or, more precisely, $\ell^2(\mathbb{Z})$) of square-summable sequences of real or complex numbers.[1] That is, ℓ^2 consists of all infinite sequences $\{\ldots, c_{-2}, c_{-1}, c_0, c_1, c_2, \ldots\}$, $c_k \in \mathbb{K}$, for which

$$\sum_{k=-\infty}^{\infty} |c_k|^2 < \infty.$$

Another example of a Hilbert space one might have seen is the space $L^2(\mathbb{R})$ of square-integrable complex-valued functions on $\mathbb{R}$, that is, of all functions[2] $f : \mathbb{R} \to \mathbb{K}$ for which

$$\int_{-\infty}^{\infty} dx\, |f(x)|^2 < \infty.$$

In view of their special nature, it may therefore come as a surprise that Hilbert spaces play a central role in many areas of mathematics, notably in analysis, but also including (differential) geometry, group theory, stochastics, and even number theory. In addition, the notion of a Hilbert space provides the mathematical foundation of quantum mechanics. Indeed, the definition of a Hilbert space was first given by von Neumann (rather than Hilbert!) in 1927 precisely for the latter purpose. However, despite his exceptional brilliance, even von Neumann would probably not have been able to do so without the preparatory work in pure mathematics by Hilbert and others, which produced numerous constructions (like the ones mentioned above) that are now regarded as examples of the abstract notion of a Hilbert space. It is quite remarkable how a particular development within pure mathematics crossed one in theoretical physics in this way; this crossing is reminiscent to the one leading to the calculus around 1670; see below. Today, the most spectacular new application of Hilbert space theory is given by Noncommutative Geometry [5], where the motivation from pure mathematics is merged with the physical input from quantum mechanics. Consequently, this is an important field of research in pure mathematics as well as in mathematical physics.

In what follows, we shall separately trace the origins of the concept of a Hilbert space in mathematics and physics. As we shall see, Hilbert space theory is part of functional analysis, an area of mathematics that emerged between approximately 1880–1930. Functional analysis is almost indistinguishable from what is sometimes called 'abstract analysis' or 'modern analysis,'

[1] In what follows, we mainly work over the reals in order to serve intuition, but many infinite-dimensional vector spaces, especially Hilbert spaces, are defined over the complex numbers. Hence we will write our formulae in a way that is correct also for $\mathbb{C}$ instead of $\mathbb{R}$. Of course, for $z \in \mathbb{R}$ the expression $|z|^2$ is just z^2. We will occasionally use the fancy letter $\mathbb{K}$, for *Körper*, which in these notes stands for either $\mathbb{K} = \mathbb{R}$ or $\mathbb{K} = \mathbb{C}$.

[2] As we shall see, the elements of $L^2(\mathbb{R})$ are, strictly speaking, not simply functions but equivalence classes of Borel functions. For detailed information we recommend the course *Maat en Integraal* by Professor A. van Rooij, which runs parallel to the present one.

which marked a break with classical analysis. The latter involves, roughly speaking, the study of properties of a single function, whereas the former deals with spaces of functions.[3] One may argue that classical analysis is tied to classical physics,[4] whereas modern analysis is associated with quantum theory. Of course, both kinds of analysis were largely driven by intrinsic mathematical arguments as well.[5] The final establishment of functional analysis and Hilbert space theory around 1930 was made possible by *combining* a concern for rigorous foundations with an interest in physical applications [3].

I.2 Origins in mathematics

Cf. [3, 6, 21, 23] for more information on the history of functional analysis and Hilbert spaces. The key idea behind functional analysis is to look at functions as points in some infinite-dimensional vector space. To appreciate the depth of this idea, it should be mentioned that the concept of a finite-dimensional vector space, today routinely taught to first-year students, only emerged in the work of Grassmann between 1844 and 1862 (to be picked up very slowly by other mathematicians because of the obscurity of Grassmann's writings), and that even the far less precise notion of a 'space' (other than a subset of $\mathbb{R}^n$) was not really known before the work of Riemann around 1850. Indeed, Riemann not only conceived the idea of a manifold (albeit in embryonic form, to be made rigorous only in the 20th century), whose points have a status comparable to points in $\mathbb{R}^n$, but also explicitly talked about spaces of functions (initially analytic ones, later also more general ones). However, Riemann's spaces of functions were not equipped with the structure of a vector space. In 1885 Weierstrass considered the distance between two functions (in the context of the calculus of variations), and in 1897 Hadamard took the crucial step of connecting the set-theoretic ideas of Cantor with the notion of a space of functions. Finally, in his PhD thesis of 1906, which is often seen as a turning point in the development of functional analysis, Hadamard's student Fréchet defined what is now called a metric space (i.e., a possibly infinite-dimensional vector space equipped with a metric, see below), and gave examples of such spaces whose points are functions.[6] After 1914, the notion of a topological space due to Hausdorff led to further progress, eventually leading to the concept of a topological vector space, which contains all spaces mentioned below as special cases.

To understand the idea of a space of functions, we first reconsider $\mathbb{R}^n$ as the space of all functions $f : \{1, 2, \ldots, n\} \to \mathbb{R}$, under the identification $x^1 = f(1), \ldots, x^n = f(n)$. Clearly, under this identification the vector space operations in $\mathbb{R}^n$ just correspond to pointwise operations on functions (e.g., $f + g$ is the function defined by $(f + g)(k) := f(k) + g(k)$, etc.). Hence $\mathbb{R}^n$ is a function space itself, consisting of functions defined on a finite set.

The given structure of $\mathbb{R}^n$ as a vector space may be enriched by defining the length $\|f\|$ of a vector f and the associated distance $d(f, g) = \|f - g\|$ between two vectors f and g. In addition,

[3] The modern concept of a function as a map $f : [a, b] \to \mathbb{R}$ was only arrived at by Dirichlet as late as 1837, following earlier work by notably Euler and Cauchy. But Newton already had an intuitive graps of this concept, at least for one variable.

[4] Classical analysis grew out of the calculus of Newton, which in turn had its roots in both geometry and physics. (Some parts of the calculus were later rediscovered by Leibniz.) In the 17th century, geometry was a practical matter involving the calculation of lenths, areas, and volumes. This was generalized by Newton into the calculus of integrals. Physics, or more precisely mechanics, on the other hand, had to do with velocities and accellerations and the like. This was abstracted by Newton into differential calculus. These two steps formed one of the most brilliant generalizations in the history of mathematics, crowned by Newton's insight that the operations of integration and differentiation are inverse to each other, so that one may speak of a unified differential and integral calculus, or briefly calculus. Attempts to extend the calculus to more than one variable and to make the ensuing machinery mathematically rigorous in the modern sense of the word led to classical analysis as we know it today. (Newton used theorems and proofs as well, but his arguments would be called "heuristic" or "intuitive" in modern mathematics.)

[5] The jump from classical to modern analysis was as discontinuous as the one from classical to quantum mechanics. The following anecdote may serve to illustrate this. G.H. Hardy was one of the masters of classical analysis and one of the most famous mathematicians altogether at the beginning of the 20th century. John von Neumann, one of the founders of modern analysis, once gave a talk on this subject at Cambridge in Hardy's presence. Hardy's comment was: "*Obviously a very intelligent man. But was that mathematics?*"

[6] Fréchet's main example was $C[a, b]$, seen as a metric space in the supremum-norm, i.e., $d(f, g) = \|f - g\|$ with $\|f\| = \sup\{f(x) \mid x \in [a, b]\}$.

the angle θ between f and g in $\mathbb{R}^n$ is defined. Lengths and angles can both be expressed through the usual inner product

$$(f,g) = \sum_{k=1}^{n} \overline{f(k)} g(k) \tag{I.1}$$

through the relations

$$\|f\| = \sqrt{(f,f)} \tag{I.2}$$

and

$$(f,g) = \|f\|\|g\| \cos\theta. \tag{I.3}$$

In particular, one has a notion of orthogonality of vectors, stating that f and g are orthogonal whenever $(f,g) = 0$, and an associated notion of orthogonality of subspaces:[7] we say that $V \subset \mathbb{R}^n$ and $W \subset \mathbb{R}^n$ are orthogonal if $(f,g) = 0$ for all $f \in V$ and $g \in W$. This, in turn, enables one to define the (orthogonal) projection of a vector on a subspace of $\mathbb{R}^n$.[8] Even the dimension n of $\mathbb{R}^n$ may be recovered from the inner product as the cardinality of an arbitrary orthogonal basis.[9]

Now replace $\{1, 2, \ldots, n\}$ by an infinite set. In this case the corresponding space of functions will obviously be infinite-dimensional in a suitable sense.[10] The simplest example is $\mathbb{N} = \{1, 2, \ldots, \}$, so that one may define $\mathbb{R}^\infty$ as the space of all functions $f : \mathbb{N} \to \mathbb{R}$, with the associated vector space structure given by pointwise operations. However, although $\mathbb{R}^\infty$ is well defined as a vector space, it turns out to be impossible to define an inner product on it, or even a length or distance. Indeed, defining

$$(f,g) = \sum_{k=1}^{\infty} \overline{f(k)} g(k) \tag{I.4}$$

it is clear that the associated length $\|f\|$ (still given by (I.2)) is infinite for most f. This is hardly surprising, since there are no growth conditions on f at infinity. The solution is to simply restrict $\mathbb{R}^\infty$ to those functions with $\|f\| < \infty$. These functions by definition form the set $\ell^2(\mathbb{N})$, which is easily seen to be a vector space. Moreover, it follows from the Cauchy–Schwarz inequality

$$(f,g) \leq \|f\|\|g\| \tag{I.5}$$

that the inner product is finite on $\ell^2(\mathbb{N})$. Consequently, the entire geometric structure of $\mathbb{R}^n$ in so far as it relies on the notions of lengths and angles (including orthogonality and orthogonal projections) is available on $\ell^2(\mathbb{N})$. Running ahead of the precise definition, we say that $\mathbb{R}^n \cong \ell^2(\{1, 2, \ldots, n\})$ is a finite-dimensional Hilbert space, whereas $\ell^2(\mathbb{N})$ is an infinite-dimensional one. Similarly, one may define $\ell^2(\mathbb{Z})$ (or indeed $\ell^2(S)$ for any countable set S) as a Hilbert space in the obvious way.

From a modern perspective, $\ell^2(\mathbb{N})$ or $\ell^2(\mathbb{Z})$ are the simplest examples of infinite-dimensional Hilbert spaces, but historically these were not the first to be found.[11] The initial motivation for the concept of a Hilbert space came from the analysis of integral equations[12] of the type

$$f(x) + \int_a^b dy\, K(x,y) f(y) = g(x), \tag{I.6}$$

[7] A subspace of a vector space is by definition a linear subspace.

[8] This is most easily done by picking a basis $\{e_i\}$ of the particular subspace V. The projection pf of f onto V is then given by $pf = \sum_i (e_i, f) e_i$.

[9] This is the same as the cardinality of an arbitrary basis, as any basis can be replaced by an orthogonal one by the Gram–Schmidt procedure.

[10] The dimension of a vector space is defined as the cardinality of some basis. The notion of a basis is complicated in general, because one has to distinguish between algebraic (or Hamel) and topological bases. Either way, the dimension of the spaces described below is infinite, though the cardinality of the infinity in question depends on the type of basis. The notion of an algebraic basis is very rarely used in the context of Hilbert spaces (and more generally Banach spaces), since the ensuing dimension is either finite or uncountable. The dimension of the spaces below with respect to a topological basis is countably infinite, and for a Hilbert space all possible cardinalities may occur as a possible dimension. In that case one may restrict oneself to an orthogonal basis.

[11] From the point of view of most mathematicians around 1900, a space like $\ell^2(\mathbb{N})$ would have been far to abstract to merit consideration.

[12] Integral equations were initially seen as reformulations of differential equations. For example, the differential equation $Df = g$ or $f'(x) = g(x)$ for unknown f is solved by $f = \int g$ or $f(x) = \int_0^x dy\, g(y) = \int_0^1 dy\, K(x,y) g(y)$ for $K(x,y) = \theta(x-y)$ (where $x \leq 1$), which is an integral equation for g.

where f, g, and K are continuous functions and f is unknown. Such equations were first studied from a somewhat modern perspective by Volterra and Fredholm around 1900, but the main breakthrough came from the work of Hilbert between 1904–1910. In particular, Hilbert succeeded in relating integral equations to an infinite-dimensional generalization of linear algebra by choosing an orthonormal basis $\{e_k\}$ of continuous functions on $[a,b]$ (such as $e_k(x) := \exp(2\pi kix)$ on the interval $[0,1]$), and defining the (generalized) Fourier coefficents of f by $\hat{f}_k := (e_k, f)$ with respect to the inner product

$$(f,g) := \int_a^b dx\, \overline{f(x)} g(x). \tag{I.7}$$

The integral equation (I.6) is then transformed into an equation of the type

$$\hat{f}_k = \sum_l \hat{K}_{kl} \hat{f}_l = \hat{g}_l. \tag{I.8}$$

Hilbert then noted from the Parseval relation (already well known at the time from Fourier analysis and more general expansions in eigenfunctions)

$$\sum_{k\in\mathbb{Z}} |\hat{f}_k|^2 = \int_a^b dx\, |f(x)|^2 \tag{I.9}$$

that the left-hand side is finite, so that $\hat{f} \in \ell^2(\mathbb{Z})$. This, then, led him and his students to study ℓ^2 also abstractly. E. Schmidt should be mentioned here in particular. Unlike Hilbert, already in 1908 he looked at ℓ^2 as a 'space' in the modern sense, thinking of seqences (c_k) as point in this space. Schmidt studied the geometry of ℓ^2 as a Hilbert space in the modern sense, that is, empasizing the inner product, orthogonality, and projections, and decisively contributed to Hilbert's work on spectral theory.

The space $L^2(a,b)$ appeared in 1907 in the work of F. Riesz[13] and Fischer as the space of (Lebesgue) integrable functions[14] on (a,b) for which

$$\int_a^b dx\, |f(x)|^2 < \infty;$$

of course, this condition holds if f is continuous on $[a,b]$. Equipped with the inner product (I.7), this was another early example of what is now called a Hilbert space.[15] The context of its appearance was what is now called the Riesz–Fischer theorem: *Given any sequence (c_k) of real (or complex) numbers and any orthonormal system (e_k) in $L^2(a,b)$,*[16] *there exists a function $f \in L^2(a,b)$ for which $(e_k, f) = c_k$ if and only if $c \in \ell^2$, i.e., if $\sum_k |c_k|^2 < \infty$.*

At the time, the Riesz–Fischer theorem was completely unexpected, as it proved that two seemingly totally different spaces were 'the same' from the right point of view. In modern terminology, the theorem establishes an isomorphism of ℓ^2 and L^2 as Hilbert spaces, but this point of view was only established twenty years later, i.e., in 1927, by von Neumann. Inspired by quantum mechanics (see below), in that year von Neumann gave the definition of a Hilbert space as an abstract mathematical structure, as follows. First, an **inner product** on a vector space V over a field $\mathbb{K}$ (where $\mathbb{K} = \mathbb{R}$ or $\mathbb{K} = \mathbb{C}$), is a map $V \times V \to \mathbb{K}$, written as $\langle f, g\rangle \mapsto (f,g)$, satisfying, for all $f, g \in V$ and $t \in \mathbb{K}$,

1. $(f,f) \geq 0$;
2. $(g,f) = \overline{(f,g)}$;

[13] Frederic Riesz had a brother, Marcel Riesz, who was a well-known mathematician too.

[14] More precisely, the elements of $L^2(a,b)$ are not functions but equivalence classes thereof, where $f \sim g$ when $\|f-g\|_2 = 0$.

[15] The term 'Hilbert space' was first used by Schoenflies in 1908 for ℓ^2, and was introduced in the abstract sense by von Neumann in 1927; see below.

[16] The notion of an orthonormal system of functions on the interval $[a,b]$ was as old as Fourier, and was defined abstractly by Hilbert in 1906.

3. $(f, tg) = t(f, g)$;
4. $(f, g + h) = (f, g) + (f, h)$;
5. $(f, f) = 0 \Rightarrow f = 0$.

Given an inner product on V, one defines an associated length function or norm (see below) $\|\cdot\| : V \to \mathbb{R}^+$ by (I.2). A **Hilbert space** (over $\mathbb{K}$) is a vector space (over $\mathbb{K}$) with inner product, with the property that Cauchy sequences with respect to the given norm are convergent (in other words, V is complete in the given norm).[17] Hilbert spaces are denoted by the letter H rather than V. Thus Hilbert spaces preserve as much as possible of the geometry of $\mathbb{R}^n$.

It can be shown that the spaces mentioned above are Hilbert spaces. Defining an **isomorphism** of Hilbert spaces $U : H_1 \to H_2$ as an invertible linear map preserving the inner product (i.e., $(Uf, Ug)_2 = (f, g)_1$ for all $f, g \in H_1$), the Riesz–Fischer theorem shows that $\ell^2(\mathbb{Z})$ and $L^2(a, b)$ are indeed isomorphic.

In a Hilbert space the inner product is fundamental, the norm being derived from it. However, one may instead take the norm as a starting point (or, even more generally, the metric, as done by Fréchet in 1906). The abstract properties of a norm were first identified by Riesz in 1918 as being satisfied by the supremum norm, and were axiomatized by Banach in his thesis in 1922. A **norm** on a vector space V over a field $\mathbb{K}$ as above is a function $\|\cdot\| : V \to \mathbb{R}^+$ with the properties:

1. $\|f + g\| \leq \|f\| + \|g\|$ for all $f, g \in V$;
2. $\|tf\| = |t|\|f\|$; for all $f \in V$ and $t \in \mathbb{K}$;
3. $\|f\| = 0 \Rightarrow f = 0$.

The usual norm on $\mathbb{R}^n$ satisfies these axioms, but there are many other possibilities, such as

$$\|f\|_p := \left(\sum_{k=1}^{n} |f(k)|^p \right)^{1/p} \tag{I.10}$$

for any $p \in \mathbb{R}$ with $1 \leq p < \infty$, or

$$\|f\|_\infty := \sup\{|f(k)|, k = 1, \ldots, n\}.$$

In the finite-dimensional case, these norms (and indeed all other norms) are all equivalent in the sense that they lead to the same criterion of convergence (technically, they generate the same topology): if we say that $f_n \to f$ when $\|f_n - f\| \to 0$ for some norm on $\mathbb{R}^n$, then this implies convergence with respect to any other norm. This is no longer the case in infinite dimension. For example, one may define $\ell^p(\mathbb{N})$ as the subspace of $\mathbb{R}^\infty$ that consists of all vectors $f \in \mathbb{R}^\infty$ for which

$$\|f\|_p := \left(\sum_{k=1}^{\infty} |f(k)|^p \right)^{1/p} \tag{I.11}$$

is finite. It can be shown that $\|\cdot\|_p$ is indeed a norm on $\ell^p(\mathbb{N})$, and that this space is complete in this norm. As with Hilbert spaces, the examples that originally motivated Riesz to give his definition were not ℓ^p spaces but the far more general L^p spaces, which he began to study in 1910. For example, $L^p(a, b)$ consists of all (equivalence classes of Lebesgue) integrable functions f on (a, b) for which

$$\|f\|_p := \left(\int_a^b dx\, |f(x)|^p \right)^{1/p} \tag{I.12}$$

[17] A sequence (f_n) is a Cauchy sequence in V when $\|f_n - f_m\| \to 0$ when $n, m \to \infty$; more precisely, for any $\varepsilon > 0$ there is $N \in \mathbb{N}$ such that $\|f_n - f_m\| < \varepsilon$ for all $n, m > N$. A sequence (f_n) converges if there is $f \in V$ such that $\lim_{n\to\infty} \|f_n - f\| = 0$.

is finite, still for $1 \leq p < \infty$, and also $\|f\|_\infty := \sup\{|f(x)|, x \in (a,b)\}$. Eventually, in 1922 Banach defined what is now called a **Banach space** as a vector space (over $\mathbb{K}$ as before) that is complete in some given norm.

Long before the abstract definitions of a Hilbert space and a Banach space were given, people began to study the infinite-dimensional generalization of functions on $\mathbb{R}^n$. In the hands of Volterra, the calculus of variations originally inspired the study of functions $\varphi : V \to \mathbb{K}$, later called **functionals**, and led to early ideas about possible continuity of such functions. However, although the calculus of variations involved nonlinear functionals as well, only linear functionals turned out to be tractable at the time (until the emergence of nonlinear functional analysis much later). Indeed, even today (continuous) linear functionals still form the main scalar-valued functions that are studied on infinite-dimensional (topological) vector spaces. For this reason, throughout this text a **functional** will denote a **continuous linear functional**. For $H = L^2(a,b)$, it was independently proved by Riesz and Fréchet in 1907 that any functional on H is of the form $g \mapsto (f,g)$ for some $f \in H$.[18] The same result for arbitrary Hilbert spaces H was written down only in 1934–35, again by Riesz, although it is not very difficult.

The second class of 'functions' on Hilbert spaces and Banach spaces that could be analyzed in detail were the generalizations of matrices on $\mathbb{R}^n$, that is, linear maps from the given space to itself. Such functions are now called operators.[19] For example, the integral equation (I.6) is then simply of the form $(1+K)f = g$, where $1 : L^2(a,b) \to L^2(a,b)$ is the identity operator $1f = f$, and $K : L^2(a,b) \to L^2(a,b)$ is the operator given by $(Kf)(x) = \int_a^b dy\, K(x,y)f(y)$. This is easy for us to write down, but in fact it took some time before integral of differential equations were interpreted in terms of operators acting on functions.[20] They managed to generalize practically all results of linear algebra to operators, notably the existence of a complete set of eigenvectors for operators of the stated type with symmetric kernel, that is, $K(x,y) = K(y,x)$.[21]

The abstract concept of a (bounded) operator (between what we now call Banach spaces) is due to Riesz in 1913. It turned out that Hilbert and Schmidt had studied a special class of operators we now call 'compact', whereas an even more famous student of Hilbert's, Weyl, had investigated a singular class of operators now called 'unbounded' in the context of ordinary differential equations. Spectral theory and eigenfunctions expansions were studied by Riesz himself for general bounded operators on Hilbert spaces (seen by him as a special case of general normed spaces), and later, more specifically in the Hilbert space case, by Hellinger and Toeplitz (culminating in their pre-von Neumann review article of 1927).

In the Hilbert space case, the results of all these authors were generalized almost beyond recognition by von Neumann in his book from 1932 [19], to whose origins we now turn.

I.3 Origins in physics

For more details on the origin of the Hilbert space concept in physics see [12, 13, 17]. For biographical information on John von Neumann[22] see [9, 10, 16, 25].

From 1900 onwards, physicists had begun to recognize that the classical physics of Newton, Maxwell and Lorentz (i.e., classical mechanics, Newtonian gravity, and electrodynamics) could not describe all of Nature. The fascinating era that was thus initiated by Planck, to be continued

[18] More generally, in 1910 Riesz showed that any functional on $L^p(a,b)$ is given by an element $L^q(a,b)$, where $1/p + 1/q = 1$, by the same formula. Since $p = 2$ implies $q = 2$, this of course implies the earlier Hilbert space result.

[19] Or *linear* operators, but for us linearity is part of the definition of an operator.

[20] For example, Hilbert and Schmidt did not really have the operator concept but (from the modern point of view) worked in terms of the associated quadratic form. That is, the operator $a : H \to H$ defines a map $q : H \times H \to \mathbb{K}$ by $\langle f, g\rangle \mapsto (f, ag)$.

[21] The associated quadratic form then satisfies $\overline{q(f,g)} = q(g,f)$.

[22] John von Neumann (1903–1957) was a Hungarian prodigy; he wrote his first mathematical paper at the age of seventeen. Except for this first paper, his early work was in set theory and the foundations of mathematics. In the Fall of 1926, he moved to Göttingen to work with Hilbert, the most prominent mathematician of his time. Around 1920, Hilbert had initiated his *Beweistheory*, an approach to the axiomatization of mathematics that was doomed to fail in view of Gödel's later work. However, at the time that von Neumann arrived, Hilbert was mainly interested in quantum mechanics; see below.

mainly by Einstein, Bohr, and De Broglie, ended in 1925–1927 with the discovery of quantum mechanics. This theory replaced classical mechanics, and was initially discovered in two guises.

First, Heisenberg discovered a form of quantum mechanics that at the time was called 'matrix mechanics.' Heisenberg's basic idea was that in atomic physics physical observables (that is, measurable quantities) should not depend on continuous variables like position and momentum (as he did not believe the concept of an electronic orbit in an atom made sense), but on discrete quantities, like the natural numbers $n = 1, 2, 3, \ldots$ labelling the orbits in Bohr's model of the atom. Specifically, Heisenberg thought that in analogy to a 'quantum jump' from one orbit to the other, everything should be expressed in terms of two such numbers. Thus he replaced the functions $f(x, p)$ of position and momentum in terms of which classical physics is formulated by quantities $f(m, n)$. In order to secure the law of conservation of energy in his new mechanics, he was forced to postulate the multiplication rule $f * g(m, n) = \sum_l f(m, l)g(l, n)$, replacing the rule $fg(x, p) = f(x, p)g(x, p)$ of classical mechanics. He noted that $f * g \neq g * f$, unlike in classical mechanics, and saw in this non-commutativity of physical observables the key revolutionary character of quantum mechanics. When he showed his work to his boss Born, a physicist who as a former assistant to Hilbert was well versed in mathematics, Born saw, after a sleepless night, that Heisenberg's multiplication rule was the same as the one known for matrices, but now of infinite size.[23] Thus Heisenberg's embryonic formulation of quantum theory, written down in 1925 in a paper generally seen as the birth of quantum mechanics, came to be known as 'matrix mechanics'.

Second, Schrödinger was led to a formulation of quantum theory called 'wave mechanics', in which the famous symbol Ψ, denoting a 'wave function,' played an important role. To summarize a long story, Schrödinger based his work on de Broglie's idea that in quantum theory a wave should be associated to each particle; this turned Einsteins's concept of a photon from 1905 on its head.[24] De Broglie's waves should, of course, satisfy some equation, similar to the fundamental wave equation or Maxwell's equations. It is this equation that Schrödinger proposed in 1926 and which is now named after him.[25] Schrödinger found his equation by studying the transition from wave optics to geometric optics, and by (wrongly) believing that there should be a similar transition from wave mechanics to classical mechanics.[26]

Thus in 1926 one had two alternative formulations of quantum mechanics, which looked completely different, but each of which could explain certain atomic phenomena. The relationship and possible equivalence between these formulations was, of course, much discussed at the time. The most obvious difficulty in relating Heisenberg's work to Schrödinger's was that the former was a theory of observables lacking the concept of a state, whereas the latter had precisely the opposite feature: Schrödinger's wave functions were states, but where were the observables? To answer this question, Schrödinger introduced his famous expressions $Q = x$ (more precisely, $Q\Psi(x) = x\Psi(x)$) and $P = -i\hbar\partial/\partial x$, defining what we now call unbounded operators on the Hilbert space $L^2(\mathbb{R}^3)$. Subsequently, Dirac, Pauli, and Schrödinger himself recognized that wave mechanics was related to matrix mechanics in the following way: Heisenberg's matrix $x(m, n)$ was nothing but the matrix element (e_n, Qe_m) of the position operator Q with respect to the orthonormal basis of $L^2(\mathbb{R}^3)$ given by the eigenfunctions of the Hamiltonian $H = P^2/2m + V(Q)$. Conversely, the vectors in ℓ^2 on which Heisenberg's matrices acted could be interpreted as states. However, these observations fell far short of an equivalence proof of wave mechanics and matrix mechanics (as is sometimes claimed), let alone of a mathematical understanding of quantum mechanics.

Heisenberg's paper was followed by the 'Dreimännerarbeit' of Born, Heisenberg, and Jordan

[23] At the time, matrices and linear algebra were unknown to practically all physicists.

[24] Einstein's revolutionary proposal, which marked the true conceptual beginning of quantum theory, had been that light, universally seen as a wave phenomenon at the time, had a particle nature as well. The idea that light consists of particles had earlier been proposed by none other than Newton, but had been discredited after the discovery of Young around 1800 (and its further elaboration by Fresnel) that light displayes interference phenomena and therefore should have a wave nature. This was subsequently confirmed by Maxwell's theory, in which light is an oscillation of the electromagnetic field. In his PhD thesis from 1924, de Broglie generalized and inverted Einstein's reasoning: where the latter had proposed that light waves are particles, the former postulated that particles are waves.

[25] He first found the time-independent Schrödinger equation $H\Psi = E\Psi$ with $H = -\hbar^2\Delta/2m+V$, and subsequently got the time-dependent one $H\Psi = i\hbar\partial\Psi/\partial t$.

[26] Technically, Schrödinger relied on the Hamilton–Jacobi formulation of classical mechanics.

(1926); all three were in Göttingen at the time. Born turned to his former teacher Hilbert for mathematical advice. Hilbert had been interested in the mathematical structure of physical theories for a long time; his Sixth Problem (1900) called for the mathematical axiomatization of physics. Aided by his assistants Nordheim and von Neumann, Hilbert ran a seminar on the mathematical structure of quantum mechanics, and the three wrote a joint paper on the subject (now obsolete).

It was von Neumann alone who, at the age of 23, recognized the mathematical structure of quantum mechanics. In this process, he defined the abstract concept of a Hilbert space discussed above; as we have said, previously only some examples of Hilbert spaces had been known. Von Neumann saw that Schrödinger's wave functions were unit vectors in the Hilbert space $L^2(\mathbb{R}^3)$, and that Heisenberg's observables were linear operators on the Hilbert space ℓ^2. The Riesz–Fischer theorem then implied the mathematical equivalence between wave mechanics and matrix mechanics. In a series of papers that appeared between 1927–1929, von Neumann defined Hilbert space, formulated quantum mechanics in this language, and developed the spectral theory of bounded as well as unbounded normal operators on a Hilbert space. This work culminated in his book [19], which to this day remains the definitive account of the mathematical structure of elementary quantum mechanics.[27]

Von Neumann proposed the following mathematical formulation of quantum mechanics. The observables of a given physical system are the self-adjoint (possibly unbounded) linear operators a on a Hilbert space H. The pure states of the system are the unit vectors in H. The expectation value of an observable a in a state ψ is given by $(\psi, a\psi)$. The transition probability between two states ψ and φ is $|(\psi, \varphi)|^2$. As we see from (I.3), this number is just $(\cos\theta)^2$, where θ is the angle between the unit vectors ψ and φ. Thus the geometry of Hilbert space has a direct physical interpretation in quantum mechanics, surely one of von Neumann's most brilliant insights. Later on, he would go beyond his Hilbert space approach to quantum theory by developing such topics and quantum logic (see [1]) and operator algebras (cf. [5]).

[27] Von Neumann's book was preceded by Dirac's *The Principles of Quantum Mechanics* (1930), which contains another brilliant, but this time mathematically questionable account of quantum mechanics in terms of linear spaces and operators.

Chapter II

Metric spaces, normed spaces, and Hilbert spaces

II.1 Basic definitions

We repeat two basic definitions from the Introduction, and add a third:

Definition II.1 *Let V be a vector space over a field $\mathbb{K}$ (where $\mathbb{K} = \mathbb{R}$ or $\mathbb{K} = \mathbb{C}$).*

An **inner product** *on V is a map $V \times V \to \mathbb{K}$, written as $\langle f, g\rangle \mapsto (f, g)$, satisfying, for all $f, g, h \in V$ and $t \in \mathbb{K}$:*

1. $(f, f) \in \mathbb{R}^+ := [0, \infty)$ *(positivity);*
2. $(g, f) = \overline{(f, g)}$ *(symmetry);*
3. $(f, tg) = t(f, g)$ *(linearity 1);*
4. $(f, g + h) = (f, g) + (f, h)$ *(linearity 2);*
5. $(f, f) = 0 \Rightarrow f = 0$ *(positive definiteness).*

A **norm** *on V is a function $\|\cdot\| : V \to \mathbb{R}^+$ satisfying, for all $f, g, h \in V$ and $t \in \mathbb{K}$:*

1. $\|f + g\| \leq \|f\| + \|g\|$ *(triangle inequality);*
2. $\|tf\| = |t|\|f\|$ *(homogeneity);*
3. $\|f\| = 0 \Rightarrow f = 0$ *(positive definiteness).*

A **metric** *on V is a function $d : V \times V \to \mathbb{R}^+$ satisfying, for all $f, g, h \in V$:*

1. $d(f, g) \leq d(f, h) + d(h, g)$ *(triangle inequality);*
2. $d(f, g) = d(g, f)$ *for all $f, g \in V$ (symmetry);*
3. $d(f, g) = 0 \Leftrightarrow f = g$ *(definiteness).*

The notion of a metric applies to any set, not necessarily to a vector space, like an inner product and a norm. These structures are related in the following way:[1]

[1] Apart from a norm, an inner product defines another structure called a **transition probability**, which is of great importance to quantum mechanics; cf. the Introduction. Abstractly, a transition probability on a set S is a function $p : S \times S \to [0, 1]$ satisfying $p(x, y) = 1 \Leftrightarrow x = y$ (cf. Property 3 of a metric) and $p(x, y) = p(y, x)$. See [14]. Now take the set S of all vectors in a complex inner product space that have norm 1, and define an equivalence relation on S by $f \sim g$ iff $f = zg$ for some $z \in \mathbb{C}$ with $|z| = 1$. (Without taking equivalence classes the first axiom would not be satisfied). The set $S = \mathsf{S}/\sim$ is then equipped with a transition probability defined by $p([f], [g]) := |(f, g)|^2$. Here $[f]$ is the equivalence class of f with $\|f\| = 1$, etc. In quantum mechanics vectors of norm 1 are (pure) states, so that the transition probability between two states is determined by their angle θ. (Recall the elementary formula from Euclidean geometry $(x, y) = \|x\|\|y\| \cos\theta$, where θ is the angle between x and y in $\mathbb{R}^n$.)

Proposition II.2 *1. An inner product on V defines a norm on V by means of $\|f\| = \sqrt{(f,f)}$.*

2. A norm on V defines a metric on V through $d(f,g) := \|f-g\|$.

The proof of this claim is an easy exercise; part 1 is based on the **Cauchy–Schwarz inequality**

$$|(f,g)| \leq \|f\|\|g\|, \tag{II.1}$$

whose proof in itself is an exercise, and part 2 is really trivial: the three axioms on a norm immediately imply the corresponding properties of the metric. The question arises when a norm comes from an inner product in the stated way: this question is answered by the **Jordan–von Neumann theorem**:

Theorem II.3 *A norm $\|\cdot\|$ on a vector space comes from an inner product through $\|f\| = \sqrt{(f,f)}$ if and only if*

$$\|f+g\|^2 + \|f-g\|^2 = 2(\|f\|^2 + \|g\|^2). \tag{II.2}$$

In that case, one has

$$4(f,g) = \|f+g\|^2 - \|f-g\|^2 \quad \text{for } \mathbb{K} = \mathbb{R}$$

and

$$4(f,g) = \|f+g\|^2 - \|f-g\|^2 + i\|f-ig\|^2 - i\|f+ig\|^2 \quad \text{for } \mathbb{K} = \mathbb{C}.$$

We leave the proof of this theorem as an exercise as well, though it is by no means trivial.

Applied to the ℓ^p and L^p spaces mentioned in the introduction, this yields the result that the norm in these spaces comes from an inner product if and only if $p = 2$; see below for a precise definition of $L^p(\Omega)$ for $\Omega \subseteq \mathbb{R}^n$. There is no (known) counterpart of this result for the transition from a norm to a metric.[2] It is very easy to find examples of metrics that do not come from a norm: on any vector space (or indeed any set) V the formula $d(f,g) = \delta_{fg}$ defines a metric not derived from a norm. Also, if d is any metric on V, then $d' = d/(1+d)$ is a metric, too: since cleary $d'(f,g) \leq 1$ for all f, g, this metric can never come from a norm.

II.2 Convergence and completeness

The reason we look at metrics in a Hilbert space course is, apart from general education, that many concepts of importance for Hilbert spaces are associated with the metric rather than with the underlying inner product or norm. The main such concept is convergence:

Definition II.4 *Let $(x_n) := \{x_n\}_{n\in\mathbb{N}}$ be a sequence in a metric space (V,d). We say that $x_n \to x$ (i.e., (x_n) converges to $x \in V$) when $\lim_{n\to\infty} d(x_n, x) = 0$, or, more precisely: for any $\varepsilon > 0$ there is $N \in \mathbb{N}$ such that $d(x_n, x) < \varepsilon$ for all $n > N$.*

In a normed space, hence in particular in a space with inner product, this therefore means that $\lim_{n\to\infty} \|x_n - x\| = 0$.[3]

A sequence (x_n) in (V,d) is called a **Cauchy sequence** when $d(x_n, x_m) \to 0$ when $n, m \to \infty$; more precisely: for any $\varepsilon > 0$ there is $N \in \mathbb{N}$ such that $d(x_n, x_m) < \varepsilon$ for all $n, m > N$. Clearly, a convergent sequence is Cauchy: from the triangle inequality and symmetry one has

$$d(x_n, x_m) \leq d(x_n, x) + d(x_m, x).$$

So for given $\varepsilon > 0$ there is $N \in \mathbb{N}$ such that $d(x_n, x) < \varepsilon/2$, etcetera. However, the converse statement does not hold in general, as is clear from the example of the metric space $(0,1)$ with metric $d(x,y) = |x-y|$: the sequence $x_n = 1/n$ does not converge in $(0,1)$ (for an example involving a vector space see the exercises). In this case one can simply extend the given space to $[0,1]$, in which every Cauchy sequence does converge.

[2] More generally, a metric (on an arbitrary set) defines a so-called topology on this set, but we leave this to the Topology course by F. Clauwens.

[3] Such convergence is sometimes called **strong convergence**, in contrast to **weak convergence**, which for an inner product space means that $\lim_n |(y, x_n - x)| = 0$ for each $y \in V$.

Definition II.5 *A metric space (V, d) is called* **complete** *when every Cauchy sequence converges.*

- *A vector space with norm that is complete in the associated metric is called a* **Banach space**.
- *A vector space with inner product that is complete in the associated metric is called a* **Hilbert space**.

Like any good definition, this one too comes with a theorem:

Theorem II.6 *For any metric space (V, d) there is a complete metric space $(\tilde{V}, \tilde{d})$ (unique up to isomorphism) containing (V, d) as a dense subspace*[4] *on which $\tilde{d} = d$. If V is a vector space, then so is $\tilde{V}$. If the metric d comes from a norm, then $\tilde{V}$ carries a norm inducing $\tilde{d}$ (so that $\tilde{V}$, being complete, is a Banach space). If the norm on V comes from an inner product, then $\tilde{V}$ carries an inner product, which induces the norm just mentioned (so that $\tilde{V}$ is a Hilbert space), and whose restriction to V is the given inner product.*

Since this theorem is well known and basic in analysis, we will not give a complete proof, but will just sketch the main idea. One defines $\tilde{V}$ as the set of all Cauchy sequences (x_n) in V, modulo the equivalence relation $(x_n) \sim (y_n)$ when $\lim_n d(x_n, y_n) = 0$. (When x_n and y_n converge in V, this means that they are equivalent when they have the same limit.) The metric $\tilde{d}$ on the set of such equivalence classes $[x_n] := [(x_n)]$ is defined by $\tilde{d}([x_n], [y_n]) := \lim_n d(x_n, y_n)$. (This limit exists, since using the triangle inequality one easily shows that $|d(x_n, y_n) - d(x_m, y_m)| \leq d(x_n, x_m) + d(y_n, y_m)$.) The embedding $\iota : V \hookrightarrow \tilde{V}$ is given by identifying $x \in V$ with the Cauchy sequence $(x_n = x \,\forall n)$, i.e., $\iota(x) = [x_n = x]$. It follows that a Cauchy sequence (x_n) in $V \subseteq \tilde{V}$ converges to $[x_n]$, for

$$\lim_m \tilde{d}(\iota(x_m), [x_n]) = \lim_m \tilde{d}([x_n = x_m], [x_n]) = \lim_m \lim_n d(x_m, x_n) = 0$$

by definition of a Cauchy sequence. Furthermore, one can show that any Cauchy sequence in $\tilde{V}$ converges by approximating its elements by elements of V.

If V is a vector space, the corresponding linear structure on $\tilde{V}$ is given by $[x_n]+[y_n] := [x_n+y_n]$ and $t[x_n] := [tx_n]$. If V has a norm, the corresponding norm on $\tilde{V}$ is given by $\|[x_n]\| := \lim_n \|x_n\|$. If V has an inner product, the corresponding inner product on $\tilde{V}$ is given by $([x_n], [y_n]) := \lim_n (x_n, y_n)$. ■

A finite-dimensional vector space is complete in any possible norm. In infinite dimensions, completeness generally depends on the norm. For example, take $V = C([0, 1])$. This space is complete in the **supremum-norm** or **sup-norm**

$$\|f\|_\infty := \sup\{f(x) \mid x \in [0, 1]\}, \tag{II.3}$$

but is incomplete in the L^2**-norm**

$$\|f\|_2 := \sqrt{(f, f)} \tag{II.4}$$

derived from the inner product

$$(f, g) := \int_0^1 dx\, \overline{f(x)} g(x). \tag{II.5}$$

The first claim follows from the theory of uniform convergence, whereas the latter follows from an explicit counterexample to completeness (exercise!).

These considerations can easily be extended to sets $\Omega \subseteq \mathbb{R}^n$.[5] First, assume that Ω is compact. The space $C(\Omega)$ is complete in the supremum-norm (defined by the obvious analogue of (II.3)), but incomplete in the L^2-norm induced from the inner product

$$(f, g) := \int_\Omega d^n x\, \overline{f(x)} g(x). \tag{II.6}$$

[4] This means that any point in $\tilde{V}$ is the limit of some convergent sequence in V with respect to the metric $\tilde{d}$.

[5] Strictly speaking, Ω should be a Borel subset of $\mathbb{R}^m$; just think of open or closed subsets, or countable intersections thereof.

To cover the noncompact case, we introduce the spaces $C_c(\Omega)$ and $C_0(\Omega)$. First, $C_c(\Omega)$ consists of all continuous functions on Ω with compact support, where the **support** of a function is defined as the smallest closed set outside which it vanishes. In other words, $C_c(\Omega)$ contains those functions that are nonzero inside some compact set. Second, $C_0(\Omega)$ consists of all continuous functions on Ω that vanish at infinity, in the sense that for each $\epsilon > 0$ there is a compact subset $K \subset \Omega$ such that $|f(x)| < \epsilon$ for all x outside K. Clearly, $C_c(\Omega) \subseteq C_0(\Omega)$, with equality $C_c(\Omega) = C_0(\Omega) = C(\Omega)$ when Ω is compact. Now, when Ω is noncompact it can be shown (by easy examples) that $C_c(\Omega)$ is not complete in the sup-norm; its completion turns out to be $C_0(\Omega)$.[6] Also, the inner product (II.6) is still defined on $C_c(\Omega)$ (but not on $C_0(\Omega)$!), which space again fails to be complete in the associated norm.

Definition II.7 *Let $\Omega \subseteq \mathbb{R}^n$.*[7] *The Hilbert space $L^2(\Omega)$ is defined as the completion of $C_c(\Omega)$ in the inner product (II.6).*

This is a fairly abstract definition of this space, as it relies on the completion procedure explained in the proof of Theorem II.6.[8]

II.3 Orthogonality

As stressed in the Introduction, Hilbert spaces are the vector spaces whose geometry is closest to that of $\mathbb{R}^3$. In particular, the inner product yields a notion of orthogonality. We say that two vectors $f, g \in H$ are **orthogonal**, written $f \perp g$, when $(f, g) = 0$.[9] Similary, two subspaces[10] $K \subset H$ and $L \subset H$ are said to be orthogonal ($K \perp L$) when $(f, g) = 0$ for all $f \in K$ and all $g \in L$. A vector f is called orthogonal to a subspace K, written $f \perp K$, when $(f, g) = 0$ for all $g \in K$, etc. We define the **orthogonal complement** $K^\perp$ of a subspace $K \subset H$ as

$$K^\perp := \{f \in H \mid f \perp K\}. \tag{II.7}$$

This set is automatically linear, so that the map $K \mapsto K^\perp$, called **orthocomplementation**, is an operation from subspaces of H to subspaces of H. Clearly, $H^\perp = 0$ and $0^\perp = H$.

Lemma II.8 *For any subspace $K \subset H$ one has $\overline{K^\perp} = \overline{K}^\perp = K^\perp$.*

If $f_n \to f$ in H, then $(f_n - f, g) \to 0 \, \forall g \in H$ by Cauchy–Schwarz. Let $g \in K$ and $f_n \in K^\perp$; it follows that $(f, g) = \lim_n (f_n, g) = 0$. Hence $f \in K^\perp$. The other equality is trivial. ∎

This lemma will be improved later on.

Recall that a basis of a finite-dimensional vector space V is a linearly independent set (e_i) such that any $v \in V$ can be written as $v = \sum_i v_i e_i$ for some $v_i \in \mathbb{K}$. In the infinite-dimensional case, we restrict ourselves to the case that V is a Banach space, and define a basis in precisely the same way, where now the sum $\sum_i v_i e_i$ may be infinite, and is meant to converge to v in norm. In other words, a basis of a Banach space V has the property that the linear span of all e_i is dense in V. We say that V is **separable** when it contains a countable dense subset; this is easily seen to be equivalent to having a countable basis. This is a pretty subtle notion: for example, $C_0(\Omega)$ is separable in the sup-norm, but $C_b(\Omega)$ (i.e., the space of all bounded continuous functions on Ω) is not.

When V is a Hilbert space, we alway require a basis (e_i) to be **orthonormal**, i.e., $(e_i, e_j) = \delta_{ij}$. Using Zorn's lemma (or the axiom of choice), it can be shown that any Hilbert space H has an

[6] For those who know some topology: this is true for any locally compact Hausdorff space Ω.

[7] Again, as a Borel subset.

[8] For those familiar with modern integration theory (i.e., in the sense of Lebesgue), a direct definition is available: $L^2(\Omega)$ consists of equivalence classes of Borel functions $f : \Omega \to \mathbb{K}$ that satisfy $\int_\Omega d^n x \, |f(x)|^2 < \infty$. The equivalence relation is $f \sim g$ when $\int_\Omega d^n x \, |f(x) - g(x)|^2 = 0$. The inner product is still given by (II.6), with two comments: Firstly, the integral is defined in the sense of Lebesgue (whereas in the main text we could use the integral in the sense of Riemann, since (II.6) was only defined for continuous functions). Secondly, the left-hand side is really $([f], [g])$ instead of (f, g).

[9] By definition of the norm, if $f \perp g$ one has Pythagoras' theorem $\|f + g\|^2 = \|f\|^2 + \|g\|^2$.

[10] Recall that a subspace of a vector space is by definition a linear subspace.

orthonormal basis. The cardinality of all bases is the same, and defines the dimension of H. However, *in this course we restrict ourselves to separable Hilbert spaces.* These are sufficient to deal with quantum mechanics and with most applications of Hilbert space theory to mathematics. For example, the spaces $L^2(\Omega)$ for (Borel) $\Omega \subset \mathbb{R}^n$ and $\ell^2(S)$ for countable S are separable. In the separable case, many arguments simplify. For example, one can prove existence of an orthonormal basis without Zorn's lemma:

Theorem II.9 *Any separable Hilbert space has an orthonormal basis.*

The proof is an exercise, based on the Gram–Schmidt procedure.

Let (e_i) by an orthonormal basis of a separable Hilbert space H. By definition, any $f \in H$ can be written as $f = \sum_i c_i e_i$. Taking the inner product with a fixed e_j, one has

$$(e_j, f) = (e_j, \lim_{N\to\infty} \sum_{i=1}^{N} c_i e_i) = \lim_{N\to\infty} c_i (e_j, e_i) = c_j.$$

Here we have assumed $N > k$, and the limit may be taken outside the inner product since if $f_n \to f$ in H then $(g, f_n) \to (g, f)$ for fixed $g \in H$, as follows from Cauchy–Schwarz. It follows that

$$f = \sum_i (e_i, f) e_i, \tag{II.8}$$

from which one obtains **Parseval's equality**

$$\sum_i |(e_i, f)|^2 = \|f\|^2. \tag{II.9}$$

Chapter III

Operators and functionals

III.1 Bounded operators

Let V be a vector space. An **operator** on V is a linear map $a : V \to V$ (i.e., $a(\lambda v + \mu w) = \lambda a(v) + \mu a(w)$ for all $\lambda, \mu \in \mathbb{K}$ and $v, w \in V$). We usually write av for $a(v)$.

Definition III.1 *If V is a normed vector space, we call an operator $a : V \to V$* **bounded** *when*

$$\|a\| := \sup \{\|av\|,\, v \in V,\, \|v\| = 1\} < \infty. \tag{III.1}$$

It easily follows that if a is bounded, then

$$\|a\| = \inf \{C \geq 0 \mid \|av\| \leq C\|v\| \; \forall v \in V\}. \tag{III.2}$$

Moreover, if a is bounded, then

$$\|av\| \;\leq\; \|a\|\, \|v\| \tag{III.3}$$

for all $v \in V$. This inequality is extremely important.[1] Another useful property, which immediately follows from (III.3), is

$$\|ab\| \leq \|a\|\|b\|. \tag{III.4}$$

Here $ab := a \circ b$, so that $(ab)(v) := a(bv)$.

When V is finite-dimensional, any operator is bounded. There are many ways to see this.[2] Indeed, let $V = \mathbb{C}^n$, so that $B(\mathbb{C}^n) = M_n(\mathbb{C})$ is the space of all complex $n \times n$ matrices. The Hilbert space norm on $\mathbb{C}^n$ is the usual one, i.e., $\|z\|^2 = \sum_{k=1}^n \overline{z}_k z_k$, and the induced norm on $M_n(\mathbb{C})$ is (III.1). As we shall see (cf. (III.14) below), $\|a\|^2$ is equal $\|a^*a\|$ (where a^* is the adjoint of a), which also coincides with the largest eigenvalue of a^*a; this is immediate from the minimax-property of eigenvalues.[3]

For an infinite-dimensional example, take $V = C_c(\mathbb{R})$, and let $a \in C(\mathbb{R})$ (with abuse of notation) define the **multiplication operator** $a_0 : C_c(\mathbb{R}) \to C_c(\mathbb{R})$ by $a_0 f(x) := a(x)f(x)$. This operator is bounded with respect to the sup-norm or the L^2-norm on $C_c(\mathbb{R})$ iff $a \in C_b(\mathbb{R})$, in other words, if $\|a\|_\infty < \infty$. For example, a_0 is not bounded when $a(x) = x$, and bounded when $a(x) = \exp(-x^2)$. Let us now pass to the closure of V in the two norms at hand. The closure of $C_c(\mathbb{R})$ in the sup-norm is $C_0(\mathbb{R})$, whereas its closure in the L^2-norm is $L^2(\mathbb{R})$. Call the resulting multiplication operator simply a. In either case, one then has $\|a\| = \|a\|_\infty$. This generalizes to any $\Omega \subseteq \mathbb{R}^n$ (exercise for compact Ω). To prove this and similar results, the following argument is very useful.

We denote the completion or closure of a subspace V_0 of a Banach space V by $\overline{V_0} \subset V$; the abstract completion of V_0 can be identified with a subspace of V_0 by identifying the equivalence class $[x_n]$ in the abstract completion procedure with the limit of (x_n) in V (check the details!).

[1] For those who know topology: it can be shown that an operator on V is bounded iff it is continuous in the topology on V derived from the norm.

[2] For topologists: any linear map $\mathbb{K}^n \to \mathbb{K}^n$ is automatically continuous, hence bounded (the continuity of the map on the unit sphere implies that the supremum in (III.1) is finite, since the unit ball in $\mathbb{K}^n$ is compact).

[3] Since a^*a is Hermitian, it has a basis of eigenvectors.

Proposition III.2 *Let $V_0 \subset V$ be a subspace of a Banach space, and let $a_0 : V_0 \to V_0$ be a bounded operator. Then there exists a unique bounded extension of a_0 to an operator $a : \overline{V_0} \to \overline{V_0}$ with the same norm as a_0. In particular, when V_0 is dense in V, the extension a is defined on all of V.*

The idea is to define ax for $x \notin V_0$ by $ax := \lim_n a_0 x_n$, where $(x_n) \subset V_0$ converges to x. We leave the easy details to the reader.[4] Hence in the above examples it suffices to compute the norm of a_0 in order to find the norm of a.

Proposition III.3 *If V is a normed vector space, then so is the set $B(V)$ of all bounded operators on V. If V is a Banach space, then so is $B(V)$.*[5]

The proof of the first claim is trivial, given (III.3). For the second claim, Let $\{a_n\}$ be a Cauchy sequence in $B(V)$. In other words, for any $\epsilon > 0$ there is a natural number $N(\epsilon)$ such that $\|a_n - a_m\| < \epsilon$ when $n, m > N(\epsilon)$. For arbitrary $v \in V$, the sequence $\{a_n v\}$ is a Cauchy sequence in V, because

$$\|a_n v - a_m v\| \leq \|a_n - a_m\| \, \|v\| \leq \epsilon \|v\| \tag{III.5}$$

for $n, m > N(\epsilon)$. Since V is complete by assumption, the sequence $\{a_n v\}$ converges to some $w \in V$. Now define a map a on V by $av := w = \lim_n a_n v$. This map is obviously linear. Taking $n \to \infty$ in (III.5), we obtain

$$\|av - a_m v\| \leq \epsilon \|v\| \tag{III.6}$$

for all $m > N(\epsilon)$ and all $v \in V$. It now follows from (III.1) that $a - a_m$ is bounded. Since $a = (a - a_m) + a_m$, and $B(V)$ is a linear space, we infer that a is bounded. Moreover, (III.6) and (III.1) imply that $\|a - a_m\| \leq \epsilon$ for all $m > N(\epsilon)$, so that $\{a_n\}$ converges to a. Since we have just seen that $a \in B(V)$, this proves that $B(V)$ is complete. ∎

III.2 Bounded functionals

The second class of functions on a vector space V worthy of study consists of **functionals**, that is, linear maps $\varphi : V \to \mathbb{K}$. The definition of boundedness of functionals defined on a normed vector space is basically the same as for operators: we say that φ is bounded when

$$\|\varphi\| := \sup \{|\varphi(v)|, \, v \in V, \, \|v\| = 1\} < \infty, \tag{III.7}$$

and as for operators we have

$$\|\varphi\| = \inf \{C \geq 0 \| \mid \varphi(v)\| \leq C \|v\| \, \forall v \in V\} \tag{III.8}$$

and, if φ is bounded,

$$\|\varphi(v)\| \leq \|\varphi\| \, \|v\| \tag{III.9}$$

for all $v \in V$.[6] Similarly, if V is a Banach space then so is the space V^* of all bounded functionals on V; this space is called the **dual** of V. Finally, the obvious analogue of Proposition III.2 holds: *if $V_0 \subset V$ is a subspace of a Banach space, and $\varphi_0 : V_0 \to \mathbb{K}$ is a bounded functional, then there*

[4] When V is a Hilbert space H, and $H_0 \subset H$, then a bounded operator $a_0 : H_0 \to H_0$ cannot merely be isometrically extended to the closure $\overline{H_0}$, but even, still isometrically, to all of H. This extension is not unique; an example is given by pap, where p is the projection onto $\overline{H_0}$. See below.

[5] Combining this result with (III.4), one arrives at the conclusion that $B(V)$ is a so-called Banach algebra. Recall that an **algebra** is a vector space with an associative bilinear operation ('multiplication') $\cdot : A \times A \to A$; we usually write ab for $a \cdot b$. It is clear that $B(V)$ is an algebra (with unit) under operator multiplication. A **Banach algebra** is a Banach space A which is at the same time an algebra, in which for all $a, b \in A$ one has (III.4). It follows that multiplication in a Banach algebra is separately continuous in each variable.

[6] As for operators, a bounded functional is automatically continuous. In fact, in the literature the term 'bounded functional' is rather unusual, to be replaced by 'continuous functional'.

exists a unique extension of φ_0 to a bounded functional $\varphi : \overline{V_0} \to \overline{V_0}$ with the same norm as φ_0. Hence when V_0 is dense in V, the extension φ is defined on V.[7]

Returning to our example $V = C_c(\mathbb{R})$, a function $a \in C(\mathbb{R})$ does not merely define an operator on V but also a functional $\varphi_a : V \to \mathbb{K}$ by the formula $\varphi_a(f) := \int_{\mathbb{R}} dx\, a(x)f(x)$. One can show (see below) that φ_a is bounded with respect to the sup-norm iff $a \in L^1(\mathbb{R})$, i.e., iff $\|a\|_1 := \int_{\mathbb{R}} dx\, |a(x)| < \infty$, with norm $\|\varphi_a\| = \|a\|_1$, whereas φ_a is bounded with respect to the L^2-norm iff $a \in L^2(\mathbb{R})$, with norm $\|\varphi_a\| = \|a\|_2$. This follows from the theorem of Riesz, in which $L^p(\Omega)$ for $\Omega \subset \mathbb{R}^n$ is defined as the completion of $C_c(\Omega)$ in the L^p-norm

$$\|f\|_p := \left(\int_\Omega d^n x\, |f(x)|^p \right)^{1/p} \tag{III.10}$$

for $1 \leq p < \infty$, and

$$\|f\|_\infty := \sup\{f(x) \mid x \in \Omega\}. \tag{III.11}$$

Theorem III.4 *Let $1 \leq p \leq \infty$. The dual of $L^p(\Omega)$ is $L^q(\Omega)$, where $\frac{1}{p} + \frac{1}{q} = 1$. The identification of $f \in L^q(\Omega)$ with an element φ_f of $L^p(\Omega)^*$ is given by $\varphi_f(g) = \int_\Omega d^n x\, f(x)g(x)$.*

We omit the proof of this theorem, as it relies on Lebesgue integration theory. We will, however, prove the Hilbert space case $p = 2$ (hence $q = 2$). Namely, this is a special case of one of the most important results on Hilbert spaces,[8] which also confirms the fact that Hilbert spaces play a unique role among general Banach spaces:

Theorem III.5 *For any Hilbert space H one has $H^* \cong H$, where for $\mathbb{K} = \mathbb{C}$ the isomorphism $H \to H^*$ is antilinear.*[9] *In other words, any $f \in H$ defines a bounded functional φ_f on H by $\varphi_f(g) = (f, g)$, and any element of H^* is of this form. Moreover, $\|\varphi_f\| = \|f\|$.*

The proof is easy. First, given $f \in H$, φ_f is bounded by Cauchy–Schwarz. Conversely, take $\varphi \in H^*$, and let N be the kernel of φ. This is a closed subspace of H by the boundedness of φ. If $N = H$ then $\varphi = 0$ so we are ready, since $\varphi = \varphi_{f=0}$. Assume $N \neq H$. Since, N is closed, $N^\perp$ is not empty, and contains h with $\|h\| = 1$.[10] For any $f \in H$, one has $\varphi(f)h - \varphi(h)f \in N$, so $(h, \varphi(f)h - \varphi(h)f) = 0$, which means $\varphi(f)(h, h) = \varphi(h)(h, f)$, or $\varphi(f) = (g, f)$ with $g = \overline{\varphi(h)}h$.

To compute $\|\varphi_f\|$, first use Cauchy–Schwarz to prove $\|\varphi_f\| \leq \|f\|$, and then apply φ_f to f to prove equality. ∎

III.3 The adjoint

Now let $V = H$ be a Hilbert space, and let $a : H \to H$ be a bounded operator. The inner product on H gives rise to a map $a \mapsto a^*$, which is familiar from linear algebra: if $H = \mathbb{K}^n$, so that, upon choosing the standard basis (e_i), a is a matrix $a = (a_{ij})$ with $a_{ij} = (e_i, ae_j)$, then the adjoint is given by $a^* = (\overline{a_{ji}})$. In other words, one has

$$(a^* f, g) = (f, ag) \tag{III.12}$$

[7] This result is completely overshadowed by the **Hahn–Banach theorem**: *For a functional φ_0 on a linear subspace V_0 of a Banach space V there exists a functional φ on V such that $\varphi = \varphi_0$ on V_0 and $\|\varphi\| = \|\varphi_0\|$. In other words, each functional defined on a linear subspace of V has an extension to V with the same norm.*

Here it is not required that V_0 be dense in V, and accordingly the extension φ is usually not unique (it is when V_0 is dense, for in that case one defines φ for $x \notin V_0$ by $\varphi(x) := \lim_n \varphi_0(x_n)$, where $(x_n) \subset V_0$ converges to x, as for operators). We omit the proof of the Hahn–Banach theorem, for it relies on the axiom of choice and is not particularly instructive. Note that this result is more general than the corresponding result for operators, as in the Hahn–Banach theorem V is not required to be a Hilbert space.

[8] As mentioned in the Introduction, this theorem is due to Riesz and Fréchet for L^2-spaces and due to Riesz in general.

[9] This means that $\lambda f \mapsto \overline{\lambda}\varphi_f$ for $\lambda \in \mathbb{C}$.

[10] Pick an orthonormal basis (e_n) of N. Since N is closed, any f of the form $f = \sum_n c_n e_n$ lies in N, $c_n \in \mathbb{K}$. Since $N \neq H$, there exists $g \notin N$, which implies that $g \neq \sum_n (e_n, g)e_n$, or $h := g - \sum_n (e_n, g)e_n \neq 0$. Clearly, $h \in N^\perp$, and since $h \neq 0$ the vector $h/\|h\|$ has norm 1.

for all $f, g \in \mathbb{K}^n$. This equation defines the adjoint also in the general case, but to prove existence of a^* Theorem III.5 is needed: for fixed $a \in B(H)$ and $f \in H$, one defines a functional $\varphi_f : H \to \mathbb{K}$ by $\varphi_f(g) := (f, ag)$. This functional is bounded by Cauchy–Schwarz and (III.3):

$$|\varphi_f(g)| = |(f, ag)| \leq \|f\|\|ag\| \leq \|f\|\|a\|\|g\|,$$

so $\|\varphi_f\| \leq \|f\|\|a\|$. Hence by Theorem III.5 there exists a unique $h \in H$ such that $\varphi_f(g) = (h, f)$ for all $g \in H$. Now, for given a the association $f \mapsto h$ is clearly linear, so that we may define $a^* : H \to H$ by $a^* f := h$, or, in other words, by (III.12). Note that the map $a \mapsto a^*$ is anti-linear: for $\mathbb{K} = \mathbb{C}$ one has $(\lambda a)^* = \overline{\lambda} a$ for $\lambda \in \mathbb{C}$. It is an easy exercise to show that for each $a \in B(H)$ one has[11]

$$\|a^*\| = \|a\| \tag{III.13}$$
$$\|a^* a\| = \|a\|^2. \tag{III.14}$$

A bounded operator $a : H \to H$ is called **self-adjoint**[12] when $a^* = a$. It immediately follows form (III.12) that for self-adjoint a one has $(f, af) \in \mathbb{R}$.[13] The most important examples of self-adjoint operators are projections.

Definition III.6 *A* **projection** *on a Hilbert space H is an operator $p \in B(H)$ satisfying $p^2 = p^* = p$.*

To understand the significance of projections, the reader should first recall the discussion about orthogonality and bases in Hilbert spaces in Chapter II.II.3. Now let $K \subset H$ be a closed subspace of H; such a subspace is a Hilbert space by itself, and therefore has an orthonormal basis (e_i). Applying (II.8) to K, it is easy to verify that

$$p : f \mapsto \sum_i (e_i, f) e_i \tag{III.15}$$

for each $f \in H$, where the sum converges in H,[14] defines a projection. Clearly,

$$pf = f \quad \text{for } f \in K;$$
$$pf = 0 \quad \text{for } f \in K^\perp. \tag{III.16}$$

Proposition III.7 *For each closed subspace $K \subset H$ one has $H = K \oplus K^\perp$. In other words, given any closed subspace $K \subset H$ each $f \in H$ has a unique decomposition $f = f^\parallel + f^\perp$, where $f^\parallel \in K$ and $f^\perp \in K^\perp$.*

The existence of the decomposition is given by $f^\parallel = pf$ and $f^\perp = (1-p)f$, and its uniqueness follows by assuming $f = g^\parallel + g^\perp$ with $g^\parallel \in K$ and $g^\perp \in K^\perp$: one then has $f^\parallel - g^\parallel = f^\perp - g^\perp$, but since the left-hand side is in K and the right-hand side is in $K^\perp$, both sides lie in $K \cap K^\perp = 0$. ■

Conversely, given a projection p, define $K := pH$. This is a closed subspace of H: if $f \in pH$ then $f = pg$ for some $g \in H$, but then $pf = p^2 g = pg = f$, so that $f \in pH$ iff $pf = f$. If $f_n \to f$ for $f_n \in pH$, then $pf = \lim_n pf_n = \lim f_n = f$, hence $f \in pH$. Furthermore, $K^\perp = (1-p)H$; verifying this fact uses both $p^* = p$ and $p^2 = p$. Defining $f^\parallel := pf$ and $f^\perp := (1-p)f$, one clearly has $f = f^\parallel + f^\perp$ with $f^\parallel \in K$ and $f^\perp \in K^\perp$, so this is the unique decomposition of f described in Proposition III.7. Hence $f^\parallel$ is given, for arbitrary $f \in H$, by both the right-hand side of (III.15) and by pf, so that (III.15) holds and p is completely characterized by its image. Hence we have proved:

[11] The second equality turns $B(H)$ into a so-called C^*-algebra. First, An abstract **involution** on an algebra A is a real-linear map $A \to A^*$ such that for all $a, b \in A$ and $\lambda \in \mathbb{C}$ one has $a^{**} = a$, $(ab)^* = b^* a^*$, and $(\lambda a)^* = \overline{\lambda} a^*$. A ***-algebra** is an algebra with an involution. A **C^*-algebra** is a Banach algebra with involution in which (III.14) holds. In addition to $B(H)$, any norm-closed subalgebra A of $B(H)$ that is also closed under the involution (i.e., if $a \in A$ then $a^* \in A$) is a C^*-algebra. Such algebras are very important throughout physics and mathematics. In fact, it has even been claimed that God is a C^*-algebra.

[12] Or **Hermitian**.

[13] In quantum mechanics self-adjoint operators model physical observables, so that these have real expectation values.

[14] The sum does not converge in the operator norm unless it is finite.

Theorem III.8 *There is a bijective correspondence $p \leftrightarrow K$ between projections p on H and closed subspaces K of H: given a projection p one puts $K := pH$, and given a closed subspace $K \subset H$ one defines p by (III.15), where (e_i) is an arbitrary orthonormal basis of K.*

An important special case is the unit operator $p = 1$, associated with $K = H$.

Corollary III.9 *For any subspace $K \subset H$ one has $K^{\perp\perp} := (K^\perp)^\perp = \overline{K}$. Hence for closed subspaces K one has $K^{\perp\perp} = K$.*

First suppose K is closed. By the previous theorem, any $f \in H$, so especially any $f \in K^{\perp\perp}$, has a unique decomposition $f = f^\parallel + f^\perp$. Since $K^{\perp\perp} = (K^\perp)^\perp$, one must have $f^\perp = 0$, hence $f = f^\parallel \in K$. So $K^{\perp\perp} \subset K$. The converse inclusion is obvious.

If K is not closed, one uses the preceding result and Lemma II.8:

$$\overline{K} = \overline{K}^{\perp\perp} = (\overline{K}^\perp)^\perp = K^{\perp\perp}. \qquad \blacksquare$$

Projections are important in many ways. One is their occurrence in the spectral theorem, which will occupy us for the remainder of the course. Furthermore, it follows from Proposition III.7 that $f \in H$ is an eigenvector of p iff $f \in pH$ or $f \in (pH)^\perp$; in the first case the eigenvector is 1, and in the second case it is 0. In quantum mechanics a projection p is a so-called **yes-no question**, in the sense that the answer to the question p is yes if the eigenvalue is 1 and no if it is 0. For general f with $(f, f) = 1$, the answer is yes with probability (f, pf) and no with probability $(f, (1-p)f) = 1 - (f, pf)$.

Apart from projections, another important class of operators on a Hilbert space consists of the unitaries. An operator $u : H \to H$ is called **unitary** when $uu^* = u^*u = 1$. Equivalently, u is **isometric**, in that $(uf, uf) = (f, f)$ for all $f \in H$, and invertible (with inverse $u^{-1} = u^*$). For example, if (e_i) and (u_i) are two orthonormal bases of H, then the operator $u(\sum_i c_i e_i) := \sum_i c_i u_i$ is unitary. In quantum mechanics, one usually encounters unitary operators of the form $u = \exp(ia)$, where a is self-adjoint and (for bounded a) the exponential is defined by its usual power series expansion, which converges in operator norm. Clearly, one has $u^* = \exp(-ia)$ and since for commuting a and b (that is, $ab = ba$) one has $\exp(a + b) = \exp(a)\exp(b)$, one sees immediately that u is indeed unitary.[15]

A **partial isometry** is an operator v for which $v^*v = p$ is a projection. A special case is an **isometry**, characterized by $p = 1$, i.e., $v^*v = 1$. An invertible isometry is clearly unitary. The structure of partial isometries is as follows.

Proposition III.10 *If v is a partial isometry, then v^* is a partial isometry as well. Let the associated projection be $q := vv^*$. The kernel of v is $(pH)^\perp$, and its range is qH. The operator v is unitary from pH to its range qH and zero on $(pH)^\perp$. Conversely, any partial isometry has this form for projections p and q.*

The proof is an exercise.

[15] In quantum mechanics the operator a is generally unbounded, a case we will deal with in great detail later on.

Chapter IV

Compact operators

IV.1 Linear algebra revisited

Compact operators on a Hilbert space (or, more generally, on a Banach space) are special bounded operators that behave like matrices on $\mathbb{K}^n$ in many ways. To make this point, we first recall the proof that any hermitian matrix (a_{ij}) (i.e., satisfying $\overline{a_{ji}} = a_{ij}$) can be diagonalized. In linear algebra this theorem is usually stated in a basis-dependent form. From our more abstract perspective of operators, the matrix (a_{ij}) arises from the operator $a : \mathbb{K}^n \to \mathbb{K}^n$ through the choice of an arbitrary orthonormal basis (e_i), in terms of which one has $a_{ij} = (e_i, ae_j)$. The spectral theorem then states that $\mathbb{K}^n$ has a (possibly) new basis of eigenvectors (u_i), in which a is diagonal: with respect to this basis one has $\tilde{a}_{ij} = (u_i, au_j) = (u_i, \lambda_j u_j) = \lambda_i \delta_{ij}$, where λ_i are the eigenvalues of a (possibly degenerate). Now, this result can be restated without any reference to the notion of a basis, as follows.

Proposition IV.1 *Let $H = \mathbb{K}^n$ be a finite-dimensional Hilbert space, and let Let $a : H \to H$ be a self-adjoint operator on H. There exists a family of mutually orthogonal projections (p_α) (i.e., $p_\alpha H \perp p_\beta H$ for $\alpha \neq \beta$, or $p_\alpha p_\beta = \delta_{\alpha\beta}$) with $\sum_\alpha p_\alpha = 1$ and $a = \sum_\alpha \lambda_\alpha p_\alpha$, where λ_α are the eigenvalues of a. In other words, p_α is the projection onto the eigenspace in H with eigenvalue λ_α; the dimension of $p_\alpha H$ is equal to the multiplicity of the eigenvalue λ_α.*

The key to the proof is the following lemma.

Lemma IV.2 *Every self-adjoint operator a on $H = \mathbb{K}^n$ has an eigenvector with associated eigenvalue λ satisfying $|\lambda| = \|a\|$.*

Note that by definition of the operator norm an eigenvalue cannot possibly be any bigger!

The proof uses some topology, but in the restricted context of $H = \mathbb{K}^n$ we simply say (Heine–Borel) that a set is compact when it is closed and bounded. We will use the following facts:

Lemma IV.3 *1. The image of a compact set in H under a continuous map into H or $\mathbb{K}$ is compact.*[1]

2. A continuous function $f : K \to \mathbb{R}$ on a compact set K attains a maximum and a minimum.

We now prove Lemma IV.2. First, the unit ball $B_1 \subset H$, defined in general by

$$B_1 := \{f \in H \mid \|f\| \leq 1\}, \tag{IV.1}$$

is clearly compact in $H = \mathbb{K}^n$. We know from basic analysis that any linear map $a : \mathbb{K}^n \to \mathbb{K}^n$ is continuous,[2] so that aB_1 is compact as well. The norm $f \mapsto \|f\|$ is continuous on H, hence

[1] This true in general: if $f : K \to Y$ is a continuous map between a compact space K and an arbitrary topological space Y, then $f(K)$ is compact in Y.

[2] A linear map $V \to V$ on a normed vector space is continuous iff it is continuous at zero. The latter easily follows for $V = \mathbb{K}^n$. The map is therefore bounded by definition (cf. (III.1)).

it follows that the function $f \mapsto \|af\|^2$ attains a maximum on B_1, say at $f = f_0$, obviously with $\|f_0\| = 1$. By definition of the norm (cf. (III.1)), this maximum must be $\|a\|^2$, so that $\|a\|^2 = \|af_0\|^2$. Cauchy–Schwarz and $a^* = a$ then yield

$$\|a\|^2 = \|af_0\|^2 = (af_0, af_0) = (f_0, a^2 f_0) \leq \|f_0\|\|a^2 f_0\| \leq \|a^2\| = \|a\|^2,$$

where we have used (III.14). In the Cauchy–Schwarz inequality (I.5) one has equality iff $g = zf$ for some $z \in \mathbb{K}$, so that we must have $a^2 f_0 = zf_0$, with $|z| = \|a\|^2$. Moreover, $z \in \mathbb{R}$, as for any self-adjoint operator eigenvalues must be real (trivial exercise!), so $a^2 f_0 = \lambda^2 f_0$ with either $\lambda = \|a\|$ or $\lambda = -\|a\|$. Now either $af_0 = \lambda f_0$, in which case the lemma is proved, or $g_0 := af_0 - \lambda f_0 \neq 0$. In the latter case,

$$ag_0 = a^2 f_0 - \lambda a f_0 = \lambda^2 f_0 - \lambda a f_0 = -\lambda g_0,$$

and the lemma follows, too. ■

Given this lemma, the proof of Proposition IV.1 is peanuts. If $(g, f_0) = 0$ then

$$(ag, f_0) = (g, a^* f_0) = (g, af_0) = \pm\lambda(g, f_0) = 0,$$

so that a maps $f_0^\perp$ into itself. In other words, if p is the projection onto $f_0^\perp$ then $pa = ap$ and $pa = pap$ is the restriction of a to $f_0^\perp = pH$. We now iterate the above procedure: we apply exactly the same reasoning to pa as an operator on pH, finding an eigenvector f_1 of pa, which of course is an eigenvector of a, as $a = pa$ on pH. We then form the orthogonal complement of f_1 in pH, etcetera. Since H is finite-dimensional, this procedure ends after n steps, leaving us with a basis $\{f_0, \ldots, f_{n-1}\}$ of H that entirely consists of eigenvectors by construction. Finally, we assemble those eigenvectors f_k with the same eigenvalue λ_α and define p_α to be the projection onto their linear span K_α (i.e., p_α is given by (II.8) applied to $K = K_\alpha$). ■

IV.2 The spectral theorem for self-adjoint compact operators

Let H be infinite-dimensional (and separable).[3] Eigenvectors and eigenvalues of operators a on a Hilbert space H are defined in the same way as for $H = \mathbb{K}^n$: if $af = \lambda f$ for some $\lambda \in \mathbb{C}$ then $f \in H$ is called an eigenvector of a with eigenvalue λ. A crucial difference with the finite- dimensional situation is that even a bounded self-adjoint operator on an infinite-dimensional Hilbert space may not have any eigenvectors (let alone a basis of them!). For example, on $H = L^2(\Omega)$ a multiplication operator defined by a nonzero continuous function has no eigenfunctions at all. The idea is now to define a class of operators on H for which the proof of Proposition IV.1 can be copied, so that the existence of a complete set of eigenvectors is guaranteed.

We will once again need some topology, but in our setting of separable Hilbert spaces we may keeps things simple: a set K in a separable Hilbert space H is **compact** when every sequence in K has a convergent subsequence, and a map $\alpha : H \to T$, where $T = \mathbb{K}$ or $T = H$, is **continuous** if it "preserves limits," i.e., if $f_n \to f$ in H then $\alpha(f_n) \to \alpha(f)$ in T.[4] For $H = \mathbb{K}^n$, this notion of compactness is equivalent to the Heine–Borel property; for separable infinite-dimensional H this equivalence no longer holds. Our notion of continuity is equivalent to the usual one in topology. The norm $f \mapsto \|f\|$ is continuous on H, which is tautological given our definition of continuity, because convergence in H has been defined in terms of the norm! I.e., $f_n \to f$ in H *means* $\|f_n - f\| \to 0$, which precisely expresses continuity of the norm. Similarly, according to our definition a bounded operator $a : H \to H$ is clearly continuous, too, for $\|af_n - af\| \to 0$ because $\|af_n - af\| \leq \|a\|\|f_n - f\|$ by (III.3). The main point is that Lemma IV.3 still applies.

Definition IV.4 *A* **compact operator** *on a Hilbert space H is a bounded operator that maps the unit ball $B_1 \subset H$ into a compact set.*

[3] The main theorem below is true in general as well, with a similar proof involving more topology.

[4] Compactness and continuity may be defined for arbitrary topological spaces in this way if one replaces sequences by nets.

This is not the case for any bounded operator, for althoug such operators are continuous, the unit ball in H is not compact.[5] If H is finite-dimensional, so that B_1 *is* compact, then any operator is compact. More generally, a finite-rank operator on an infinite-dimensional Hilbert space (i.e., an operator whose image is finite-dimensional) is compact.

Proposition IV.5 *A bounded operator on a separable Hilbert space is compact iff it is the norm-limit of a sequence of finite-rank operators.*

The proof is left as an exercise, as is the following consequence of the proposition.

Corollary IV.6 *1. If a is compact then so is its adjoint a^*;*

2. If a is compact and b is bounded then ab and ba are compact;

3. A projection p is compact iff it is finite-dimensional.

Using this corollary, it is easy to show that the set of all compact operators in $B(H)$ is a Banach space called $B_0(H)$ in the operator norm. Moreover, $B_0(H)$ is even an algebra under operator multiplication, closed under involution.[6]

Integral operators form an important class of compact operators. Without proof we mention that if $\Omega \subset \mathbb{R}^n$ is compact, any operator of the form $af(x) = \int_\Omega d^n x\, a(x,y) f(y)$ is compact when the kernel $a(-,-)$ is continuous on $\Omega \times \Omega$. More generally, for any $\Omega \subset \mathbb{R}^n$ such an operator is compact when $a(-,-) \in L^2(\Omega \times \Omega)$, i.e., when $\int d^n x d^n y\, |a(x,y)|^2 < \infty$. The following theorem completely characterizes self-adjoint compact operators.

Theorem IV.7 *Let a be a self-adjoint compact operator on a Hilbert space H. Then H has an orthonormal basis (e_i) of eigenvectors of a, in terms of which*

$$a = \sum_i \lambda_i p_i, \tag{IV.2}$$

where p_i projects onto the span of e_i, and the sum converges in the sense that $af = \sum_i \lambda_i p_i f$ for each fixed $f \in H$. Moreover, the set (λ_i) of eigenvalues of a has the property that

$$\lim_{i \to \infty} |\lambda_i| = 0. \tag{IV.3}$$

Conversely, a bounded self-adjoint operator on H of the form (IV.2) where the eigenvalues satisfy (IV.3) is compact.

To prove the first claim, we may simply repeat the proof of Proposition IV.1, as compact operators have been defined for precisely this purpose! In particular, Lemma IV.2 still holds. However, the infinite-dimensional situation makes one big difference: the iteration procedure in the proof is not a priori guaranteed to converge. To settle this, let $p = \sum_i p_i$ (with convergence as understoof in (II.8)) be the projection onto the subspace of H spanned by all eigenvectors of a. Clearly, a maps pH onto itself, and using $a^* = a$, it follows that it maps $(pH)^\perp$ onto itself as well: if $g \in (pH)^\perp$ then by definition $(f,g) = 0$ for all $f \in pH$, so $(f, ag) = (a^* f, g) = (af, g) = 0$. But $(pH)^\perp$ is a Hilbert space in its own right, and since the restriction of a to $(pH)^\perp$ is given by $(1-p)a$, this restriction is still compact by Corollary IV.6.2. Hence Lemma IV.2 applies to it, implying that $(1-p)a$ has an eigenvector in $(pH)^\perp$, which is the same as saying that a has an eigenvector in $(pH)^\perp$. This contradicts the definition of pH.

We leave the proof of the second claim as an exercise. ■

[5] The unit ball in an infinite-dimensional Hilbert space is not compact in the topology defined by the norm, in which $f_n \to f$ when $\|f_n - f\| \to 0$. Miraculously, the unit ball *is* compact in another topology, namely the so-called weak topology, in which $f_n \to f$ when $|(g, f_n - f)| \to 0$ for each fixed $g \in H$.

[6] Hence $B_0(H)$ is a C^*-algebra; see footnote 11.

Corollary IV.8 *Each eigenvalue of a self-adjoint compact operator except possibly 0 has finite multiplicity, and 0 is the only possibly accumulation point of the set of eigenvalues. Hence we may rewrite (IV.2) as*

$$a = \sum_\alpha \lambda_\alpha p_\alpha, \tag{IV.4}$$

where all eigenvalues λ_α are different and p_α is the finite-dimensional projection $p_\alpha := \sum_{i|\lambda_i=\lambda_\alpha} e_i$.

This expansion has the advantage over (IV.2) that it is unique; in (IV.2) there is an arbitrariness in the choice of basis within the eigenspace of each eigenvalue with multiplicity greater than one. In particular, the eigenvalues (λ_i) are uniquely determined by a.

Corollary IV.9 *An arbitrary compact operator a on a Hilbert space H has an expansion*

$$af = \sum_i \mu_i (e_i, f) u_i, \tag{IV.5}$$

where (e_i) and (u_i) are orthonormal bases of H, $\mu_i > 0$, and (μ_i^2) are the eigenvalues of a^*a.

Since a^*a is self-adjoint, Theorem IV.7 applies, i.e.,

$$a^*af = \sum_i \lambda_i (e_i, f) e_i. \tag{IV.6}$$

Since a^*a is positive, in the sense that $(f, a^*af) \geq 0$ for all $f \in H$ (for $(f, a^*af) = \|af\|^2$), it follows that $\lambda_i \geq 0$ for each i. Hence $\mu_i = \sqrt{\lambda_i}$ is well defined as the positive square-root. Now define $u_i := \mu_i^{-1} a e_i$. Using (II.8), eq. (IV.5) is immediate. ∎

The μ_i are sometimes called the **singular values** of a.

IV.3 Trace-class and Hilbert–Schmidt operators

Trace-class operators are special compact operators, which are of fundamental importance for quantum mechanics (see Chapter VII below). More generally, for $1 \leq p < \infty$ one defines the **Schatten class** $B_p(H)$ as the subset of $B_0(H)$ consisting of all compact operator for which

$$\|a\|_p := \left(\sum_i \mu_i^p \right)^{1/p} < \infty. \tag{IV.7}$$

Here the μ_i are the singular values of a, as just explained. As the notation suggests, $\|\cdot\|_p$ is a norm on the linear space $B_p(H)$, which is even complete in this norm (and hence is a Banach space in its own right. Note that (except when H is finite-dimensional) $B_p(H)$ is *not* complete in the operator norm $\|\cdot\|$; in fact the completion of $B_p(H)$ in $\|\cdot\|$ is precisely $B_0(H)$. It is an exercise to prove the fundamental inequality

$$\|a\| \leq \|a\|_p. \tag{IV.8}$$

This is initially defined for for $a \in B_0(H)$, but if one defines $\|a\|_p = \infty$ for $a \in B(H)$ whenever $a \notin B_0(H)$, it is valid for any bounded operator. Each $B_p(H)$ is an ideal in both $B_0(H)$ and in $B(H)$, since, as is easily shown, $ab \in B_p(H)$ if $a \in B_p(H)$ and $b \in B(H)$, or vice versa.

The Schatten classes play an important role in noncommutative geometry for any p [5], but for us the most important special cases are $p = 1$ and $p = 2$. An element of $B_1(H)$ is called a **trace-class operator**, and an element of $B_2(H)$ is called a **Hilbert–Schmidt operator**. For $a \in B_1(H)$ we define the **trace** of a by

$$\mathrm{Tr}\, a := \sum_i (e_i, a e_i), \tag{IV.9}$$

where (e_i) is an arbitrary orthonormal basis of H. It is easy to show that (IV.9) is absolutely convergent and independent of the basis (exercise). Indeed, defining $|a|$ for $a \in B_0(H)$ by

$$|a|f := \sum_i \mu_i (e_i, f) e_i, \tag{IV.10}$$

where (e_i) and (λ_i) are defined by (IV.6) and $\mu_i := \sqrt{\lambda_i}$, as before, one has

$$\|a\|_1 = Tr|a|. \tag{IV.11}$$

In fact, the so-called **absolute value** $|a|$ of a is defined for any bounded operator (see exercises), and even for any closed unbounded operator. In any case, for $a \in B_1(H)$ and $b \in B(H)$, or vice versa one has

$$\mathrm{Tr}\, ab = \mathrm{Tr}\, ba, \tag{IV.12}$$

which implies

$$\mathrm{Tr}\, uau^* = \mathrm{Tr}\, a \tag{IV.13}$$

for $a \in B_1(H)$ and u unitary. For $a \notin B_1(H)$, the trace is *not defined*, not even when it so happens that $\sum_i (e_i, ae_i) < \infty$ in some orthonormal basis; in that case, the sum will not be absolutely convergent, and might be infinite in most other bases. In particular, trace-class operators are necessarily compact and therefore have discrete spectrum (cf. Chapter VI).

Similarly, if $a \in B_2(H)$, one has

$$\|a\|_2^2 = \mathrm{Tr}\, a^*a = \sum_i \|ae_i\|^2, \tag{IV.14}$$

for any orthonormal basis (e_i). In fact, $B_2(H)$ is a Hilbert space in the inner product

$$(a, b) := \mathrm{Tr}\, a^*b; \tag{IV.15}$$

this expression is finite by positivity (i.e., $\mathrm{Tr}\, a^*a \geq 0$) and Cauchy–Schwarz. The associated norm is precisely $\|\cdot\|_2$.

The significance of $B_1(H)$ in part comes from the following fundamental result. Following the convention in quantum mechanics, we will generically denote trace-class operators by ρ.

Theorem IV.10 *Identifying $\rho \in B_1(H)$ with a functional on $B_0(H)$ by $\rho : a \mapsto \mathrm{Tr}\, \rho a$, one has*

$$B_0(H)^* \cong B_1(H). \tag{IV.16}$$

Identifying $a \in B(H)$ with a functional on $B_1(H)$ by $a : \rho \mapsto \mathrm{Tr}\, \rho a$, one has

$$B_1(H)^* \cong B(H). \tag{IV.17}$$

Both isomorphisms are isometric bijections between Banach spaces.

Since the proof uses several results we have not discussed, we merely sketch it (see [20] for a complete proof). The crucial inequality is

$$|\mathrm{Tr}\, \rho a| \leq \|\rho\|_1 \|a\|, \tag{IV.18}$$

where $\rho \in B_1(H)$ and $a \in B(H)$. This immediately implies $B_1(H) \subseteq B_0(H)^*$ and $B(H) \subseteq B_1(H)^*$, under the given identifications. Furthermore, one has

$$\|a\|_2 \leq \|a\|_1 \tag{IV.19}$$

and hence $B_1(H) \subset B_2(H)$.

To prove the inclusion $B_0(H)^* \subset B_1(H)$, we fix $\omega \in B_0(H)^*$. By definition, one has $|\omega(a)\| \leq C\|a\|$. Picking $a \in B_2(H)$ and using (IV.8) for $p = 2$, this yields $|\omega(a)\| \leq C\|a\|_2$. Since $B_2(H)$ is a Hilbert space, by the Riesz–Fréchet theorem one has $\omega(a) = (b, a) = \mathrm{Tr}\, ba$ for some $b \in B_2(H)$.

Further analysis, using the fact that ω must have an extension from $B_2(H)$ to $B_0(H)$, refines this to $b \in B_1(H)$. Then put $\rho = b^*$.

To prove the inclusion $B_1(H)^* \subset B(H)$, we fix $\omega \in B_1(H)^*$. By definition, one has $|\omega(\rho)\| \leq C\|\rho\|_1$. We now choose ρ to be of the special form $\rho = |f\rangle\langle g|$, where $f, g \in H$ and $|f\rangle\langle g|h := (g,h)f$. Such operators are trace-class with $\||f\rangle\langle g|\|_1 = \|f\|\|g\|$. Defining a quadratic form q on H (i.e., a sesquilinear map $q : H \times H \to \mathbb{C}$) by $q(f,g) := \omega(|f\rangle\langle g|)$, we have $|q(f,g)| \leq C\|f\|\|g\|$. Such quadratic forms are said to be bounded, and the fundamental theorem on bounded quadratic forms states that there is a unique bounded operator a such that $q(f,g) = (g, af)$. But for any $a \in B(H)$ and $f, g \in H$ we have $(g, af) = \mathrm{Tr}\,|f\rangle\langle g|a$; to see this, evaluate the trace in an orthonormal basis containing a vector proportional to g. Hence $\omega(\rho) = \mathrm{Tr}\,\rho a$ for ρ of the special form $\rho = |f\rangle\langle g|$. But the span of such operators is dense in $B_1(H)$, so that ω has the stated form for any $\rho \in B_1(H)$.

Chapter V

Closed unbounded operators

V.1 The closure

We are now familiar with two classes of operators on a Hilbert space: *bounded* ones, and *compact* ones. As we have seen, the latter are precisely those bounded operators for which a spectral theory analogous to that for matrices exists. It would be possible to develop the spectral theory of general bounded (self-adjoint)operators at this point, but in fact it turns out that this theory can be written down almost without extra effort for the far wider class of *closed* (self-adjoint) operators. Such operators need not be bounded, and "It is a fact of life that many of the most important operators which occur in mathematical physics are not bounded" [22].

To come to grips with the notion of un unbounded operator, let us use the definition of continuity in the preceding chapter to prove:

Theorem V.1 *An operator on a Hilbert space is bounded iff it is continuous.*

Let $a : H \to H$ be bounded. By (III.3), if $f_n \to f$ in H, that is, $\|f_n - f\| \to 0$, then $af_n \to af$ in H, since $\|af_n - af\| \leq \|a\|\|f_n - f\|$. Conversely, if a is not bounded, then for each $n \in N$ there is $f_n \in H$ with $\|f_n\| = 1$ and $\|af_n\| \geq n$. The sequence $(g_n = f_n/n)$ converges to 0, but since $\|ag_n\| \geq 1$, the sequence (ag_n) does not converge to $a0 = 0$. Hence a is not continuous, and the implication "continuous $\Rightarrow$ bounded" has been proved by *reductio ad absurdum.* ■

It follows that unbounded operators are discontinuous: if $f_n \to f$ it is not guaranteed that $af_n \to af$; indeed, it is not guaranteed that (af_n) converges at all! Hence an essential difference between the bounded and the unbounded case is that whereas for bounded operators a Proposition III.2 states that even if a is initially defined on some dense subspace D of H, it can uniquely be extended to H by continuity, for unbounded operators a such an extension by continuity will not in general exist. Although a discontinuous extension to H might exist, in practice it is very unusual to talk about unbounded operators a defined on H. This is because interesting unbounded operators tend to be defined on $D \subset H$ by some natural expression, which simply does not make sense on all of H. Consequently, the specification of the subspace D on which a is defined, called the **domain** of a, denoted by $D(a)$ is absolutely essential when a is an unbounded operator. *Unless explicitly stated otherwise, we always assume that the domain of an operator is dense in H* (otherwise, we replace H by the closure of the domain in question).

For example, we have seen that $a \in C(\mathbb{R})$ defines a bounded operator on $H = L^2(\mathbb{R})$ by multiplication when $\|f\|_\infty < \infty$, i.e., when a is bounded. When a is unbounded as a function, we cannot really make the natural claim that consequently a is unbounded as a multiplication operator on H, since a does not map H to itself as soon as it is unbounded. What we can say, however, is that a is unbounded as a multiplication operator on the subspace $D(a) = C_c(\mathbb{R})$, which (by our definition of L^2) is dense in H. Other examples are given by differential operators: whereas one cannnot really say that $a = id/dx$ is unbounded on $L^2(\mathbb{R})$ since the derivative of most functions in L^2 is not even defined,[1] one can say that a is unbounded on, say, $D(a) = C_c^1(\mathbb{R}) := C_c(\mathbb{R}) \cap C^1(\mathbb{R})$.

[1] Unless one is familiar with the theory of distributions.

There is some flexibility in the choice of the domain, and the theory of unbounded operators of closable type even largely revolves around the business of enlarging a given domain. Here we define an **extension** of a given operator $a : D(a) \to H$ as an operator $a_1 : D(a_1) \to H$ where $D(a) \subset D(a_1)$ and $a_1 = a$ on $D(a)$; we write $a \subset a_1$. As we have seen, if a is bounded there is only one interesting extension, namely the one defined on any larger domain (including H) by continuity, but in the unbounded case the theory of extension of operators turns out to be very rich indeed. As a rather trivial example, we could have defined $a = id/dx$ initially on $D(a) = C_c^\infty(\mathbb{R}) := C_c(\mathbb{R}) \cap C^\infty(\mathbb{R})$; the same expression $a_1 = id/dx$ but now defined on $D(a_1) = C_c^1(\mathbb{R})$ is formally an extension of a. Similarly, an unbounded mutliplication operator $a \in C(\mathbb{R})$ may initially be defined on $D(a) = C_c^\infty(\mathbb{R})$, to be extended by the same expression defined on $D(a_1) = C_c(\mathbb{R})$, as above. Clearly, the largest possible domain on which a multiplication operator $a \in C(\Omega)$ can be defined in the natural way is[2]

$$D(a) = \{f \in L^2(\Omega) \mid af \in L^2(\Omega)\}. \tag{V.1}$$

The particular unbounded operators that one can deal with satisfy a relic of continuity. To explain this, we define the **graph** of a as the subset $\{f, af\} \subset H \times H$. To define the notion of closedness in $H \times H$ we equip this set with the structure of a Hilbert space in the following way: we first equip $H \times H$ with the structure of a vector space by defining $\langle f_1, f_2\rangle + \langle g_1, g_2\rangle := \langle f_1 + g_1, f_2 + g_2\rangle$ and $\lambda\langle f_1, f_2\rangle := \langle \lambda f_1, \lambda f_2\rangle$, and subsequently putting an inner product on it by $(\langle f_1, f_2\rangle, \langle g_1, g_2\rangle) := (f_1, g_1) + (f_2, g_2)$. With this structure, $H \times H$ is a Hilbert space called $H \oplus H$, for it is precisely the direct sum of H with itself.

Definition V.2 *A* **closed operator** $a : D(a) \to H$ *is a linear map from a dense subspace* $D(a) \subset H$ *to* H *for which either of the following equivalent conditions holds:*

- *If* $f_n \to f$ *in* H *for a sequence* (f_n) *in* $D(a)$ *and* (af_n) *converges in* H*, then* $f \in D(a)$ *and* $af_n \to af$ *in* H*.*
- *The graph of* a *is closed.*
- *The domain* $D(a)$ *is closed in the norm* $\|f\|_a^2 := \|f\|^2 + \|af\|^2$*.*

Note that the norm $\|\cdot\|_a$ comes from the new inner product $(f, g)_a := (f, g) + (af, ag)$ on $D(a)$. Hence $D(a)$ is a Hilbert space in the new inner product when a is closed.

It is quite unusual for an operator to be closed in the form initially given. For example, a multiplication operator a in $L^2(\Omega)$ is not closed on $C_c^\infty(\Omega)$ or even on $C_c(\Omega)$; as proved below, a turns out to be closed only on the domein (V.1). Fortunately, an operator a that is not closed may often be extended into a closed one. The condition for this to be possible is as follows.

Definition V.3 *A* **closable operator** $a : D(a) \to H$ *is a linear map from a dense subspace* $D(a) \subset H$ *to* H *with the property that the closure* $G(a)^-$ *of its graph is itself the graph* $G(a^-)$ *of some operator* a^- *(called the* **closure** *of* a*).*

In other words, a^- is a closed extension of a. It is clear that a^- is uniquely defined by its graph $G(a^-) = G(a)^-$.

Proposition V.4 *An operator* a *is closable iff either of the following equivalent conditions holds:*

- *If* $f_n \to 0$ *for a sequence* (f_n) *in* $D(a)$ *and if* (af_n) *converges, then* (af_n) *must converge to 0.*
- *The closure* $G(a)^-$ *of the graph of* a *does not contain any element of the form* $(0, g)$ *for* $g \neq 0$*.*

In that case, the domain of the closure a^- *of* a *is the set of all* $f \in H$ *to which some sequence* (f_n) *in* $D(a)$ *converges and for which* (af_n) *converges as well. Its action is given by* $a^- f := \lim_n af_n$*.*

Finally, the operator a^- *is the smallest closed extension of* a*.*

[2]Similarly, the largest possible domain on which $\partial/\partial x^i$ can be defined in the natural way is $D(\partial/\partial x^i) = \{f \in L^2(\Omega) \mid \partial f/\partial x^i \in L^2(\Omega)\}$, where the derivative is defined in the distributional sense.

To verify that a^- is indeed closed, suppose $f_n \to f$ and $af_n \to g$, with (f_n) in $D(a^-)$. Since $f_n \in D(a^-)$ for fixed n, there exists $(f_{m,n})$ in $D(a)$ such that $\lim_m f_{m,n} = f_n$ and $\lim_m af_{m,n} =: g_n$ exists. Then clearly $\lim_{m,n} f_{m,n} = f$, and we claim that

$$\lim_{m,n} af_{m,n} = g. \tag{V.2}$$

Namely, $\|af_{m,n} - g\| \leq \|af_{m,n} - af_n\| + \|af_n - g\|$. For $\epsilon > 0$ take n so that the second term is $< \epsilon/2$. For that fixed n, $a(f_{m,n} - f_n)$ converges as $m \to \infty$ because $af_{m,n} \to g_n$ and af_n is independent of m. Also, recall that $f_{m,n} - f_n \to 0$ as $m \to \infty$. By assumption, a is closable, hence by definition one must have $a(f_{m,n} - f_n) \to 0$ in m. Hence we may find m so that $\|af_{m,n} - af_n\| < \epsilon/2$, so that $\|af_{m,n} - g\| < \epsilon$, and (V.2) follows. Hence $f \in D(a^-)$. Finally, since $a^-f := \lim_{m,n} af_{m,n}$ one has $a^-f = g$ by (V.2), or $a^-f = \lim_n af_n$ by definition of g. It follows that a^- is closed. This extension of a is clearly the minimal closed one.

This argument shows that for a^- to be closed it is sufficient that a is closable. Conversely, if a fails to be closable it cannot have any closed extension whatsoever, since a^- is by definition linear, and $a^-0 = 0$ for any operator. The second condition for closability is then clearly equivalent to the first. ■

For example, a multiplication operator a in $H = L^2(\Omega)$ is closable on both $D(a) = C_c^\infty(\Omega)$ and $C_c(\Omega)$: in both cases the closure has domain (V.1). On the other hand, an example of a non-closable operator is given by $H = L^2(\Omega)$, $D(a) = C_c(\Omega)$, and $af := f(0)g$, where $g \in H$ is arbitrary (cf. the exercises).

In general, even closed unbounded operators may have closed extensions, a phenomenon which is particular important in connection with the theory of self-adjointness; see below.

This section would not be complete without mentioning a special case of one of the most famous theorems in functional analysis, namely the **closed graph theorem** (for Hilbert spaces):

Theorem V.5 *If $a : H \to H$ has a closed graph, then it is bounded. In other words, a closed operator defined on all of H is necessarily bounded.*

We will use this theorem only once, since in applications an operator defined on H is usually already known to be bounded, whereas unbounded operators are never defined on H, so that their graph cannot be studied in any case.[3]

V.2 Symmetric and self-adjoint operators

The most important closed operators, not just for quantum mechanics also but for mathematics as a whole, are the self-adjoint ones. To define these, we first recall the definition of the adjoint a^* of a bounded operator $a : H \to H$. If we initially define the domain $D(a^*)$ of a^* as the set of all $f \in H$ for which the functional $g \mapsto \varphi_f(g) := (f, ag)$ is bounded, then the boundedness of a implies that $D(a^*) = H$, and we may define a^* by (III.12), i.e., $(a^*f, g) = (f, ag)$. Requiring this equality for all $g \in H$ defines a^*f uniquely: for we may take $g = e_i$ to be a basis vector, so that $a^*f = \sum_i (f, ae_i)e_i$ by (II.8). This argument show that the vector a^*f (and hence the operator a^*, since $f \in H$ is arbitrary) is even uniquely defined by (III.12) when g runs over a dense subspace in H.[4]

Definition V.6 *The adjoint a^* of an unbounded operator $a : D(a) \to H$ has domain $D(a^*)$ consisting of all $f \in H$ for which the functional $g \mapsto \varphi_f(g) := (f, ag)$ is bounded. On this domain, a^* is defined by requiring $(a^*f, g) = (f, ag)$ for all $g \in D(a)$.*

[3] On the theoretical side, however, an important consequence of the closed graph theorem is another famous result known as the **open mapping theorem**: a bounded surjective operator on a Hilbert space H is open (in that the image of an open set in H is open; the boundedness of H implies the opposite, namely that the inverse image of an open set in H is open).

[4] This can be seen in many ways. For example, any dense subspace D contains a basis of H, as can be proved in the separable case by the Gram–Schmidt procedure (and in general follows from Zorn's Lemma). Alternatively, even if $e_i \notin D$, the coefficient (h, e_i) can be computed by approximating e_i by elements in D, since by Cauchy–Schwarz one has $(h, e_i) = \lim_n (h, f_n^{(i)})$ for any sequence $f_n^{(i)} \to e_i$ in D.

Here the vector a^*f exists by the Riesz–Fréchet theorem III.5, and it is uniquely determined by our standing assumption that $D(a)$ be dense in H. However, this time we cannot conclude that $D(a^*) = H$, as in the bounded case. Indeed, it may even happen that $D(a^*)$ is zero! (See exercises.) However, this is pretty pathological, and in most 'natural' examples $D(a^*)$ turns out to be dense. For example, a multiplication operator $a \in C(\Omega)$ on $H = L^2(\Omega)$, defined on any of the domains we have considered (i.e., $D(a) = C_c^\infty(\Omega)$, $D(a) = C_c(\Omega)$, or (V.1)), has $a^* = \overline{a}$ (i.e., the complex conjugate of a seen as a multiplication operator) defined on $D(a^*)$ given by the right-hand side of (V.1). The following important result shows when $D(a^*)$ is dense.

Proposition V.7 *Let $a : D(a) \to H$ (where $D(a)$ is dense) be an operator on a Hilbert space H.*

1. *The adjoint a^* is closed.*
2. *The operator a is closable iff $D(a^*)$ is dense.*
3. *In that case, one has $a^- = a^{**}$ and $(a^-)^* = a^*$.*

The proof can be elegantly given in terms of the graph $G(a)$. Defining $U : H \oplus H \to H \oplus H$ by $U(f,g) := (g,-f)$, it is easy to verify that (exercise!)

$$G(a^*) = U(G(a)^\perp) = U(G(a))^\perp. \tag{V.3}$$

Hence the first claim immediately follows, since any orthogonal complement is closed (cf. Lemma II.8).

By Corollary (III.9) and (V.3) one has $G(a)^- = G(a)^{\perp\perp} = (U^{-1}G(a^*))^\perp$. But

$$(U^{-1}G(a^*))^\perp = \{\langle f,g\rangle \in H \oplus H \mid (f,a^*h) - (g,h) = 0 \; \forall h \in D(a^*)\}.$$

Consequently, referring to Proposition V.4, $(0,g) \in G(a)^-$ iff $g \in D(a^*)^\perp$, proving the second claim. Using (V.3) twice (first for a^*, then for a), we have

$$G(a^{**}) = (UG(a^*))^\perp = (U^2(G(a)^\perp))^\perp = G(a)^{\perp\perp} = G(a)^- = G(a^-),$$

where we have used $U^2 = -1$ and $-G(b) = G(b)$ for any operator b. This proves the first part of the third claim. Finally, if a is closable, then using (V.3) and Lemma II.8 and (V.3) once more, we have

$$G(a^*) = U(G(a)^\perp) = U((G(a)^-)^\perp) = U(G(a^-)^\perp) = G((a^-)^*). \qquad \blacksquare$$

We now come to the central definition of this chapter. An equality $a = b$ between unbounded operators always stand for $D(a) = D(b)$ and $a = b$. Similarly, $a \subset b$ means $D(a) \subset D(b)$ and $b = a$ on $D(a)$.

Definition V.8 *Let $a : D(a) \to H$ (where $D(a)$ is dense) be an operator on a Hilbert space H.*

- *If $a = a^*$, i.e., if $D(a^*) = D(a)$ and $(af,g) = (f,ag)$ for all $f,g \in D(a)$, then a is called* **self-adjoint**.
- *If $a^{**} = a^*$ (equivalently, if a is closable and $a^- = a^*$ or $(a^-)^* = a^*$), then a is called* **essentially self-adjoint**.
- *If $a \subset a^*$ i.e., if $(af,g) = (f,ag)$ for all $f,g \in D(a)$, then a is called* **symmetric**.

It follows Proposition V.7 that a self-adjoint operator is closed, and that a symmetric operator is closable (because $D(a^*)$, containing $D(a)$, is dense). For a symmetric operator one has $a \subseteq a^- = a^{**} \subseteq a^*$, with equality at the first position when a is closed, and equality at the second position when a is essentially self-adjoint; when both equalities hold, a is self-adjoint. Conversely, an essentially self-adjoint operator is, of course, symmetric. A symmetric operator may or may not have self-adjoint extensions; we will deal with this problem in detail later on. Without proof we quote the **Hellinger–Toeplitz theorem**: *If a is self-adjoint on $D(a) = H$, then a is bounded.* This confirms the idea that it is pointless to try to define unbounded operators on all of H in some manifestly discontinuous way. All this is very subtle, but the following example illustrates at least the easy part of the theory:

Proposition V.9 *A real-valued multiplication operator $a \in C(\Omega)$ on $H = L^2(\Omega)$ is essentially self-adjoint on $D(a) = C_c^\infty(\Omega)$ and on $D(a) = C_c(\Omega)$, and is self-adjoint on $D(a) = \{f \in L^2(\Omega) \mid af \in L^2(\Omega)\}$.*

Cf. (V.1)). Of course, $D(a) = H$ when $\|a\|_\infty < \infty$, since in that case a is a bounded operator, as we have seen.[5] The proof is almost trivial: by definition, $D(a^*)$ consists of all $f \in L^2(\Omega)$ for wich the functional $g \mapsto (f, ag) = \int_\Omega d^n x\, \overline{f}(x)a(x)g(x)$ is bounded; for each of the three choices of $D(a)$ listed this implies $\overline{f}a \in L^2(\Omega)$ by Riesz–Fréchet, so that $D(a^*) = \{f \in L^2(\Omega) \mid af \in L^2(\Omega)\}$, with $a^* = \overline{a}$ as a multiplication operator. If a is real-valued, then a^* is self-adjoint by the very same argument, which implies all claims. ■

A more difficult example is provided by $H = L^2([0,1])$ and $a = -id/dx$; see Section VIII.2 in [22] for the detailed analysis leading to the claims now made. Partial integration shows that a is symmetric on the domain $D(a) = \{f \in C^1([0,1]) \mid f(0) = f(1) = 0\}$, which is easy. It is more difficult to prove that the adjoint of a with respect to this domain is $a^* = -id/dx$ defined on the domain

$$D(a^*) = \{f \in AC([0,1]) \mid df/dx \in L^2([0,1])\}. \tag{V.4}$$

Here $AC([0,1])$ (where AC stands for 'absolutely continuous') consists of all functions of the type $f(x) = \int_0^x g(x)$ with $g \in L^1([0,1])$. It turns out that a^- is given by $a^- = -id/dx$ on $D(a^-) = \{f \in D(a^*) \mid f(0) = f(1) = 0\}$ (hence a is not closed). Since $D(a^-) \neq D(a^*)$, a is not essentially self-adjoint. It turns out that a has a family $(a_\theta)_{\theta \in [0,2\pi)}$ of self-adjoint extensions, defined by $a_\theta = -id/dx$ on the domain $D(a_\theta) = \{f \in D(a^*) \mid f(1) = \exp(i\theta)f(0)\}$.

[5] This result may be extended to multiplication operators defined by Lebesgue-measurable functions $a : \Omega \to \mathbb{R}$. Defining the **essential supremum** of such a function by $\|a\|_\infty^{ess} : \inf\{C \mid |a(x)| \leq C \text{ for almost every } x \in \Omega\}$, one has $a \in B(L^2(\Omega))$ iff $\|a\|_\infty^{ess} < \infty$, in that case with $\|a\| = \|a\|_\infty^{ess}$, and Proposition V.9 being valid as it stands.

Chapter VI

Spectral theory for closed unbounded operators

Until further notice, we now assume that $\mathbb{K} = \mathbb{C}$. We denote the kernel or null space of a map a by $N(a)$ and its range or image by $R(a)$. As before, $D(a)$ denotes the domain of a. Also, $a - z$ for $z \in \mathbb{C}$ denotes the operator $a - z1$.

VI.1 Resolvent and spectrum

The theory of the spectrum of a closed operator on a Hilbert space (which may be bounded or unbounded) is a generalization of the theory of eigenvalues of a matrix. From linear algebra we recall:

Proposition VI.1 *Let $a : \mathbb{C}^n \to \mathbb{C}^n$ be a linear map. The a is injective iff it is surjective.*

This follows from the fundamental fact that if $a : V \to W$ is a lnear map between vector spaces, one has $R(a) \cong V/N(a)$. If $V = W = \mathbb{C}^n$, one one count dimensions to infer that $\dim(R(a)) = n - \dim(N(a))$. Surjectivity of a yields $\dim(R(a)) = n$, hence $\dim(N(a)) = 0$, hence $N(a) = 0$, and vice versa.[1] ∎

Corollary VI.2 *Let $a : \mathbb{C}^n \to \mathbb{C}^n$ be a linear map. Then $a - z$ is invertible (i.e., injective and surjective) iff z is not an eigenvalue of a, i.e., if there exists no $f \in \mathbb{C}^n$ such that $af = zf$.*

Defining the **spectrum** $\sigma(a)$ of $a : \mathbb{C}^n \to \mathbb{C}^n$ as the set of eigenvalues of a and the **resolvent** $\rho(a)$ as the set of all $z \in \mathbb{C}$ for which $a - z$ is invertible, we therefore have

$$\sigma(a) = \mathbb{C} \backslash \rho(a). \tag{VI.1}$$

If $z \in \rho(a)$, the equation $(a - z)f = g$ for the unknown $f \in \mathbb{C}^n$ has a unique solution for any g; existence follows from the surjectivity of $a - z$, whereas uniqueness follows from its injectivity (if $a - z$ fails to be injective then any element of its kernel can be added to a given solution).

Now, if a is an operator on an infinite-dimensional Hilbert space, it may not have any eigenvalues, even when it is bounded and self-adjoint. For example, if $a(x) = \exp(-x^2)$ the associated multiplication operator $a : L^2(\mathbb{R}) \to L^2(\mathbb{R})$ is bounded and self-adjoint, but it has no eigenvalues at all: the equation $af = \lambda f$ for eigenvectors is $\exp(-x^2)f(x) = \lambda f(x)$ for (almost) all $x \in \mathbb{R}$, which holds only if f is nonzero at a single point. But in that case $f = 0$ as an element of L^2. However,

[1] In general, this proposition yields the very simplest case of the Atiyah–Singer index theorem, for which these authors received the Abel Prize in 2004. We define the **index** of a linear map $a : V \to W$ as $\mathrm{index}(a) := \dim(\ker(a)) - \dim(\mathrm{coker}(a))$, where $\ker(a) = N(a)$ and $\mathrm{coker}(a) := W/R(a)$, provided both quantities are finite. If V and W are finite-dimensional, Proposition VI.1 yields $\mathrm{index}(a) = \dim(V) - \dim(W)$; in particular, if $V = W$ then $\mathrm{index}(a) = 0$ for any linear map a. In general, the index theorem expresses the index of an operator in terms of topological data; in this simple case the only such data are the dimensions of V and W.

the situation is not hopeless. More generally, let any $a \in C_b(\mathbb{R})$, interpreted as a multiplication operator $a : L^2(\mathbb{R}) \to L^2(\mathbb{R})$. If $x_0 \in \mathbb{R}$ one may find approximate eigenvectors of a in the following sense: take

$$f_n(x) := (n/\pi)^{1/4} e^{-n(x-x_0)^2/2}. \tag{VI.2}$$

Then $\|f_n\| = 1$ and $\lim_{n\to\infty}(a(x) - a(x_0))f_n = 0$, although the sequence f_n itself has no limit in $L^2(\mathbb{R})$. Thus we may call $\lambda = a(x_0)$ something like a generalized eigenvalue of a for any $x_0 \in \mathbb{R}$, and define the spectrum accordingly: let $a : D(a) \to H$ be a (possibly unbounded) operator on a Hilbert space. We say that $\lambda \in \sigma(a)$ when there exists a sequence (f_n) in $D(a)$ for which $\|f_n\| = 1$ and

$$\lim_{n\to\infty}(a - \lambda)f_n = 0. \tag{VI.3}$$

Of course, when λ is an eigenvalue of a with eigenvector f, we may take $f_n = f$ for all n.

However, this is not the official definition of the spectrum, which is as follows.

Definition VI.3 *Let $a : D(a) \to H$ be a (possibly unbounded) operator on a Hilbert space. The* **resolvent** *$\rho(a)$ is the set of all $z \in \mathbb{C}$ for which $a - z : D(a) \to H$ is injective and surjective (i.e., invertible). The* **spectrum** *$\sigma(a)$ of a is defined by $\sigma(a) := \mathbb{C}\backslash\rho(a)$.*

Hence the *property* (VI.1) has been turned into a definition! We will prove the equivalence of this definition of the spectrum with the definition above later on. In the example just given, one has $\sigma(a) = a(\mathbb{R})$ if the right domain of a is used, namely (V.1). Thus the spectrum can be nonempty even if there aren't any eigenvalues. The subsequent theory shows that these are precisely the right definitons for spectral theory.

The following result explains the role of closedness.[2]

Proposition VI.4 *If an operator $a : D(a) \to R(a) = H$ has an inverse, then a^{-1} is bounded iff a is closed.*

The proof consists of two steps. First, one has that $a : D(a) \to R(a)$ is closed iff a^{-1} is closed. To prove "$\Rightarrow$", assume $g_n \to g$ and $a^{-1}g_n \to f$. Call $f_n := a^{-1}g_n$; then $af_n = g_n \to g$, so if a is closed then by definition $f \in D(a)$ and $af_n \to af$, so $af = g$, hence $f = a^{-1}g$, which means $a^{-1}g_n \to a^{-1}g$. In particular, $g \in R(a) = D(a^{-1})$, and it follows that a^{-1} is closed. The proof of "$\Leftarrow$" is the same, with a and a^{-1} interchanged. Geometrically, the graph of a^{-1} is just the image of the graph of a in $H \oplus H$ under the map $(f, g) \mapsto (g, f)$, hence if one is closed then so is the other.

Secondly, if $R(a) = H$, then $D(a) = H$, hence a^{-1} is bounded by the closed graph theorem (Theorem V.5). ∎

Returning to the equation $(a - z)f = g$, it now follows that when $z \in \rho(a)$, the solution f depends continuously on the initial data g iff a is closed. To avoid pathologies, we therefore assume that a is closed in what follows. Furthermore, as we shall see, practically every argument below breaks down when $(a-z)^{-1}$ is unbounded. This also explains why as far as spectral theory is concerned there isn't much difference between bounded operators and closed unbounded operators: in both cases $(a - z)^{-1}$ is bounded for $z \in \rho(a)$.

As an exercise, one easily shows that for closed a one has

$$\rho(a^*) = \overline{\rho(a)}; \quad \sigma(a^*) = \overline{\sigma(a)}. \tag{VI.4}$$

Theorem VI.5 *Let a be a closed operator.*

1. *$\rho(a)$ is open (and hence $\sigma(a)$ is closed) in $\mathbb{C}$.*
2. *The operator-valued function $z \mapsto (a - z)^{-1}$ is analytic on $\rho(a)$, i.e., it can be expressed as a norm-convergent power series in z.*

[2]Some books define the resolvent of a as the set of those $z \in \mathbb{C}$ for which $(a - z)$ is invertible *and* has bounded inverse. In that case, the resolvent is empty when a is not closed.

Everything will follow from the following lemma, in which $a \in B(H)$ is not the same a as in the theorem!

Lemma VI.6 *When $\|a\| < 1$ the sum $\sum_{k=0}^{n} a^k$ converges in norm to $(1-a)^{-1}$.*

We first show that the sum is a Cauchy sequence. Indeed, for $n > m$ one has

$$\|\sum_{k=0}^{n} a^k - \sum_{k=0}^{m} a^k\| = \|\sum_{k=m+1}^{n} a^k\| \leq \sum_{k=m+1}^{n} \|a^k\| \leq \sum_{k=m+1}^{n} \|a\|^k.$$

For $n, m \to \infty$ this goes to 0 by the theory of the geometric series. Since $B(H)$ is complete, the Cauchy sequence $\sum_{k=0}^{n} a^k$ converges for $n \to \infty$. Now compute

$$\sum_{k=0}^{n} a^k(1-a) = \sum_{k=0}^{n}(a^k - a^{k+1}) = 1 - a^{n+1}.$$

Hence

$$\|1 - \sum_{k=0}^{n} a^k(1-a)\| = \|a^{n+1}\| \leq \|a\|^{n+1},$$

which $\to 0$ for $n \to \infty$, as $\|a\| < 1$ by assumption. Thus

$$\lim_{n\to\infty} \sum_{k=0}^{n} a^k(1-a) = 1.$$

By a similar argument,

$$\lim_{n\to\infty} (1-a) \sum_{k=0}^{n} a^k = 1.$$

so that, by continuity of multiplication of bounded operators (see (III.4)) one finally has

$$\lim_{n\to\infty} \sum_{k=0}^{n} a^k = (1-a)^{-1}. \qquad \blacksquare$$

Now let a be as in Theorem VI.5. Given $z_0 \in \rho(a)$, take the open set of all $z \in \mathbb{C}$ for which $|z - z_0|\|(a-z_0)^{-1}\| < 1$. Consequently,

$$(a-z_0)^{-1} \sum_{k=0}^{\infty} \left(\frac{z-z_0}{a-z_0}\right)^k = (a-z_0)^{-1} \left(1 - (z-z_0)(a-z_0)^{-1}\right)^{-1} = (a - z_0 + (z_0 - z))^{-1} = (a-z)^{-1}.$$

This proves existence of $(a-z)^{-1}$, so that $z \in \rho(a)$, which must therefore be open. Furthermore, it follows from the same calculation that $(a-z)^{-1}$ is analytic in z. $\blacksquare$

Note that, as for ordinary (i.e., $\mathbb{C}$-valued) analytic functions, analyticity implies continuity: with

$$\|(a-z)^{-1} - (a-z_0)^{-1}\| = \|\sum_{k=1}^{\infty} \left(\frac{z-z_0}{a-z_0}\right)^k\| \leq |z-z_0|\|(a-z_0)^{-1}\|^2 \sum_{k=2}^{\infty} |z-z_0|^k \|(a-z_0)^{-1}\|^k,$$

still assuming that $|(z-z_0|\|(a-z_0)^{-1}\| < 1$, one sees that $\lim_{z\to z_0}(a-z)^{-1} = (z-z_0)^{-1}$.

The following theorem is quite remarkable, since it shows that the norm of a bounded operator on a Hilbert space is given purely algebraically, namely in terms of the spectrum.

Theorem VI.7 *If a is bounded, then $\sigma(a)$ is compact. Defining the* **spectral radius** *of a by*

$$r(a) := \sup\{|z|, z \in \sigma(a)\}, \tag{VI.5}$$

one has

$$\|a\| = r(a) \tag{VI.6}$$

when $a^* = a$, and

$$\|a\| = \sqrt{r(a^*a)} \tag{VI.7}$$

in general.

We will not prove this theorem here, as it is typical for bounded operators and our main interest in this course is in unbounded ones.[3] It clearly implies that the spectrum of a bounded self-adjoint operator is never empty, and in fact we show in a different way that the spectrum of any bounded operator on a Hilbert space is not empty:

Theorem VI.8 *If $a \in B(H)$, then $\sigma(z) \neq \emptyset$.*

The idea of the proof is that when $\sigma(z) = \emptyset$ the operator-valued function $z \mapsto (a-z)^{-1}$, which we call g from now on, is not merely analytic on $\rho(a) = \mathbb{C}$ by Theorem VI.5, but in addition vanishes at infinity. Namely, for $z \neq 0$ we write $\|g(z)\| = |z|^{-1}\|(1-a/z)^{-1}\|$ and observe that $\lim_{z\to\infty} 1 - a/z = 1$, since $\lim_{z\to\infty} \|a/z\| = 0$. Hence $\lim_{z\to\infty}(1-a/z)^{-1} = 1$, and

$$\lim_{z\to\infty} \|g(z)\| = 0. \tag{VI.8}$$

Since g is analytic and hence continuous, it follows that it is uniformly bounded (in z with respect to the operator norm). There is an operator-valued analogue of Liouville's theorem from complex analysis: any uniformly bounded analytic function on $\mathbb{C}$ taking values in the space of all bounded operators on some Banach space is constant. By (VI.8) this constant is zero, so that $g = 0$. This is absurd, so that $\rho(a) \neq \mathbb{C}$ hence $\sigma(a) \neq \emptyset$. ■

On the other hand, for unbounded operators the spectrum can (literally) be any subset of $\mathbb{C}$, including the empty set. The following example, continuing the example at the end of the previous chapter, describes some fairly unexpected possibilities.

Proposition VI.9 *Let $H = L^2([0,1])$ and $a = -id/dx : D(a) \to H$ as a formal expression, with domain to be specified below.*

- *If $D(a) = \{f \in AC([0,1]) \mid f' \in L^2 \,\&\, f(0) = 0\}$ or $D(a) = \{f \in AC([0,1]) \mid f' \in L^2 \,\&\, f(1) = 0\}$, then $\sigma(a) = \emptyset$.*
- *If $D(a) = \{f \in AC([0,1]) \mid f' \in L^2 \,\&\, f(0) = f(1) = 0\}$, then $\sigma(a) = \mathbb{C}$.*
- *$D(a) = \{f \in AC([0,1]) \mid f' \in L^2 \,\&\, f(0) = f(1)\}$, then $\sigma(a) = 2\pi\mathbb{Z}$.*

Note that a is closed in all cases. In the first it is not symmetric, in the second it is symmetric, and in the third it is self-adjoint.

If $z \in \rho(a)$, the differential equation

$$(-id/dx - z)g(x) = f(x) \tag{VI.9}$$

should have a solution $g \in D(a)$ for any $f \in H$, where the solution is obtained from f by a bounded operator. This yields

$$g(x) = e^{izx}\left(\int_0^x dt\, e^{-izt} f(t) + \int_0^1 dt\, h(t) f(t)\right),$$

where $h \in H$ is arbitrary (and independent of f) in so far as (VI.9) is solved; it should be chosen so as to satisfy the boundary condition inherent in $D(a)$. Completing the argument is an exercise. ■

VI.2 The spectrum of self-adjoint operators

For a general closed operator a, we may decompose the spectrum as

$$\sigma(a) = \sigma_d(a) \cup \sigma_c(a), \tag{VI.10}$$

where the **discrete spectrum** $\sigma_d(a)$ consists of all eigenvalues of a, and the **continuous spectrum** $\sigma_c(a)$ is the remainder of $\sigma(a)$. Recall that eigenvalues lie in $\sigma(a)$, for if $(a-\lambda)f = 0$ for some nonzero f then $a - \lambda$ cannot be injective. The spectrum of self-adjoint operators has a particularly transparent structure.

[3] See Weidmann Vol. I Ch. V or [15] for a proof.

Theorem VI.10 *Let a be a self-adjoint operator (i.e., $a^* = a$), and let $z \in \mathbb{C}$. Then one of the following possibilities occurs:*

1. *$R(a-z) = H$ iff $z \in \rho(a)$;*
2. *$R(a-z)^- = H$ but $R(a-z) \neq H$ iff $z \in \sigma_c(a)$;*
3. *$R(a-z)^- \neq H$ iff $z \in \sigma_d(a)$.*

The key to the proof is a very simple result.

Lemma VI.11 *If a is closable (equivalently, if $D(a^*)$ is dense), then $R(a-z)^- = N(a^* - \overline{z})^\perp$ and $N(a^* - \overline{z}) = R(a-z)^\perp$.*

Note that the kernel of a closed operator (in this case $a^* - \overline{z}$) is automatically closed. Easy calculations using the definition of a^* yield the inclusions $R(a-z)^\perp \subset N(a^* - \overline{z})$ and $R(a-z) \subset N(a^* - \overline{z})^\perp$. Since $K^{\perp\perp} = K^-$ for any linear subspace K of a Hilbert space, and $K \subset L$ implies $L^\perp \subset K^\perp$, the claim follows. ∎

We first prove Theorem VI.10 for $z \in \mathbb{R}$. If $R(a-z)^- \neq H$, then $N(a-z) = R(a-z)^\perp \neq 0$, so $(a-\lambda)f = 0$ has a nonzero solution and $\lambda \in \sigma_d(a)$. The converse implication has the same proof. If $R(a-z)^- = H$, then $N(a-z) = 0$ and $a - z$ is injective. Now if $R(a-z) = H$ then $a - z$ is surjective as well, and $z \in \rho(a)$. The converse is trivial given the definition of the resolvent. If $R(a-z) \neq H$, then $z \in \sigma_c(a)$ by definition of the continuous spectrum. Conversely, if $z \in \sigma_c(a)$ then $z \notin \sigma_d(a)$ and $z \notin \rho(a)$, so that $R(a-z) = H$ and $R(a-z)^- \neq H$ are exlcuded by the previous 'iff' results for $\rho(a)$ and $\sigma_d(a)$. Hence $R(a-z)^- = H$ but $R(a-z) \neq H$.

To prove Theorem VI.10 for $z \in \mathbb{C}\backslash\mathbb{R}$, we first note that eigenvalues of self-adjoint operators must be real; this is immediate since if $a^* = a$ then $\overline{(f, af)} = (af, f) = (f, af)$, so if f is an eigenvector with eigenvector λ it follows that $\overline{\lambda} = \lambda$. In fact, we will prove that if $z \in \mathbb{C}\backslash\mathbb{R}$, then also $z \in \rho_c(a)$ is impossible, so that $z \in \rho(a)$. To see this we need some lemma's.

Lemma VI.12 *Let a be symmetric. Then $\|(a-z)f\| \geq |\mathrm{Im}\,(z)|\|f\|$.*

Reading Cauchy–Schwarz in the wrong order, we obtain

$$\|(a-z)f\|\|f\| \geq |(f,(a-z)f)| = |(r - i\mathrm{Im}\,(z))\|f\|^2| \geq |\mathrm{Im}\,(z)|\|f\|^2.$$

Here we used the fact that $r := (f, af) - \mathrm{Re}\,(z)$ is a real number by virtue of the symmetry of a. ∎

Hence $z \in \mathbb{C}\backslash\mathbb{R}$ implies $N(a - \overline{z}) = 0$. Combining this with Lemma VI.11, we infer that $R(a-z)^- = N(a-\overline{z})^\perp = H$. To infer that actually $R(a-z) = H$ we need yet another lemma.

Lemma VI.13 *Let a be any densely defined operator. If $\|af\| \geq C\|f\|$ for some $C > 0$ and all $f \in D(a)$, then a is injective and $a^{-1} : R(a) \to D(a)$ is bounded with bound $\|a^{-1}\| \leq C^{-1}$.*

Injectivity is trivial, for $af = 0$ cannot have any nonzero solutions given the bound; a linear map a is injective when $af = 0$ implies $f = 0$. For the second claim, note that

$$\|a^{-1}\| = \sup\{\|a^{-1}g\|, g \in D(a^{-1}) = R(a), \|g\| = 1\} =$$

$$\sup\left\{\left\|a^{-1}\frac{af}{\|af\|}\right\|, f \in D(a), f \neq 0\right\} = \sup\left\{\left\|\frac{f}{\|af\|}\right\|, f \in D(a), f \neq 0\right\}.$$

This yields the claim. ∎

Combining this with Lemma VI.12, we see that $z \in \mathbb{C}\backslash\mathbb{R}$ implies $(a-z)^{-1} : D((a-z)^{-1}) \to D(a-z) = D(a)$ is bounded, where $D((a-z)^{-1}) = R(a-z)$. To infer that in fact $R(a-z) = H$, we use:

Lemma VI.14 *If b is closed and injective, then $b^{-1} : R(b) \to D(b)$ is closed.*

See the proof of Proposition VI.4. ■

Lemma VI.15 *If b is closed and bounded, then $D(b)$ is closed.*

This is immediate from the definition of closedness. ■

Taking $b = (a - z)^{-1}$, we find that $D((a - z)^{-1})$ is closed. Since we know that $R(a - z)^- = H$, we conclude that $R(a - z) = H$. The same is true for $\overline{z}$. Hence by Lemma VI.11, $N(a - z) = R(a - \overline{z})^\perp = H^\perp = 0$ and $a - z$ is injective. With $a - z$ already known to be surjective, $z \in \rho(a)$.

The proof of the converse implications is the same as for $z \in \mathbb{R}$, and we have finished the proof of Theorem VI.10. ■

Using similar arguments, one can prove

Theorem VI.16 *Let a be a symmetric operator. Then the following properties are equivalent:*

1. *$a^* = a$, i.e., a is self-adjoint;*
2. *a is closed and $N(a^* \pm i) = 0$;*
3. *$R(a \pm i) = H$;*
4. *$R(a - z) = H$ for all $z \in \mathbb{C}\backslash\mathbb{R}$;*
5. *$\sigma(a) \subset \mathbb{R}$.*

Similarly, the following properties are equivalent:

1. *$a^* = a^{**}$, i.e., a is essentially self-adjoint;*
2. *$N(a^* \pm i) = 0$;*
3. *$R(a \pm i)^- = H$;*
4. *$R(a - z)^- = H$ for all $z \in \mathbb{C}\backslash\mathbb{R}$;*
5. *$\sigma(a^-) \subset \mathbb{R}$.*

The second half of the theorem easily follows from the first, on which we will therefore concentrate. The implications $1 \Rightarrow 2$, $1 \Rightarrow 4$, $1 \Rightarrow 5$ and $2 \Rightarrow 3$ are immediate either from Theorem VI.10 or from its proof. The implications $4 \Rightarrow 3$ and $5 \Rightarrow 4$ are trivial. Thus it only remains to prove $3 \Rightarrow 1$.

To do so, assume $R(a \pm i) = H$. For given $f \in D(a^*)$ there must then be a $g \in H$ such that $(a^* - i)f = (a - i)g$. Since a is symmetric, we have $D(a) \subset D(a^*)$, so $f - g \in D(a^*)$, and $(a^* - i)(f - g) = 0$. But $N(a^* - i) = R(a + i)^\perp$ by Lemma VI.11, so $N(a^* - i) = 0$. Hence $f = g$, and in particular $f \in D(a)$ and hence $D(a^*) \subset D(a)$. Since we already know the opposite inclusion, we have $D(a^*) = D(a)$. Given symmetry, this implies $a^* = a$. ■

As an illustration of Theorem VI.16, one can directly show:

Proposition VI.17 *Let $a \in C(\Omega)$ define a real-valued multiplication operator on*

$$D(a) = \{f \in L^2(\Omega) \mid af \in L^2(\Omega)\} \subset H = L^2(\Omega),$$

so that $a^* = a$ (cf. Proposition V.9.) Then the operator a is injective iff $a(x) \neq 0$ for all $x \in \Omega$, and surjective iff there exists $\varepsilon > 0$ so that $|a(x)| \geq \varepsilon$ for all $x \in \Omega$; in that case a is injective and has bounded inverse. Consequently, $\sigma(a) = a(\Omega)^-$, with $a(\Omega) := \{a(x), x \in \Omega\}$.

Finally, we justify our earlier heuristic definition of the spectrum; the thrust of the theorem lies in its characterization of the continuous spectrum, of course.

Theorem VI.18 *Let a be self-adjoint. Then $\lambda \in \sigma(a)$ iff there exists a sequence (f_n) in $D(a)$ with $\|f_n\| = 1$ for all n such that $\lim_n (a - \lambda)f_n = 0$.*

Suppose $\lambda \in \sigma(a)$. If $\lambda \in \sigma_d(a)$ we are ready, taking $f_n = f$ for all n. If $\lambda \in \sigma_c(a)$, then $R(a-\lambda)^- = H$ but $R(a-\lambda) \neq H$ by Theorem VI.10. Now a is self-adjoint, hence a and $a-\lambda$ are closed, so that also $(a-\lambda)^{-1}$ is closed by Lemma VI.14. Hence $(a-\lambda)^{-1} : R(a-\lambda) \to H$ must be a a densely defined unbounded operator by Lemma VI.15, for if it were bounded then its domain would be closed, which $D((a-\lambda)^{-1}) = R(a-\lambda)$ is not, as we have just shown. Thus there is a sequence g_n in $D((a-\lambda)^{-1})$ with norm 1 and $\|(a-\lambda)^{-1}g_n\| \to \infty$. Then $f_n := (a-\lambda)^{-1}g_n/\|(a-\lambda)^{-1}g_n\|$ has the desired property.

Conversely, if $\lambda \in \rho(a)$ then $(a-\lambda)^{-1}$ is bounded, hence $(a-\lambda)f_n \to 0$ implies $f_n \to 0$, so the sequence (f_n) cannot exist, and $\lambda \in \sigma(a)$ by *reductio ad absurdum*. ■

Chapter VII

Quantum mechanics and Hilbert space

We are now going to apply the previous machinery to quantum mechanics, referring to the Introduction for history and motivation. The mathematical formalism of quantum mechanics is easier to understand if it is compared with classical mechanics, of which it is a modification. We therefore start with a rapid overview of the latter, emphasizing its mathematical structure.[1]

VII.1 Classical mechanics

The formalism of classical mechanics is based on the notions of **phase space** and **time-evolution**, going back to Descartes and Newton, and brought into its modern form by Hamilton. The phase space of a given physical system is a collection of points, each of which is interpreted as a possible state of the system.[2] At each instance of time, a given state is supposed to completely characterize the 'state of affairs' of the system, in that:

1. The value of any observable (i.e., any question that may possibly be asked about the system, such as the value of its energy, or angular momentum,...) is determined by it.[3]

2. Together with the equations of motion, the state at $t = 0$ is the only required ingredient for the prediction of the future of the system.[4]

In general, the phase space M in classical mechanics is a so-called symplectic manifold. Observables are then given by (preferably smooth) functions on M. In these notes we only look at the special case $M = \mathbb{R}^{2n}$, which describes a physical system consisting of a point particles moving in $\mathbb{R}^n$. We use coordinates $(q, p) := (q^i, p_i)$, where $i = 1, \ldots, n$. The q variable ("position") denotes the position of the particle, whereas the meaning of the p variable ("momentum") depends on the time-evolution of the system. For example, for a free particle of mass m one has the relation $\vec{p} = m\vec{v}$, where v is the velocity of the particle (see below). Let us note that one may look at, say, q^i also as an observable: seen as a function on M, one simply has $q^i(q, p) = q^i$, etc.

Given the phase space M, the specification of the system is completed by specifying a (usually smooth) function h on M, called the **Hamiltonian** of the system. For $M = \mathbb{R}^{2n}$ we therefore have h as a function of (q, p), informally written as $h = h(q, p)$. The Hamiltonian plays a dual role: it

[1] A more complete treatment should await a new course *Symplectic Geometry and Classical Mechanics*.

[2] More precisely, as a pure state; see section VII.5 below.

[3] Philosophers would say that any quantity pertaining to the system *supervenes* on its states; this means that no change in a given quantity is possibly without a change in the state. For example, most scientists would agree that the mind supervenes on the brain (seen as a physical system).

[4] We do not say that such a prediction is always possible; see below. But *if* it is possible at all, it merely requires the state and the equations of motion.

gives the value of the energy, and determines the time-evolution of the system. Indeed, given h the time-evolution is determined by **Hamilton's equations**

$$\begin{aligned} \dot{q}^i := \frac{dq^i}{dt} &= \frac{\partial h}{\partial p_i}; \\ \dot{p}_i := \frac{dp_i}{dt} &= -\frac{\partial h}{\partial q^i}. \end{aligned} \tag{VII.1}$$

For example, a particle with mass m moving in a potential V has Hamiltonian

$$h(q,p) = \frac{p^2}{2m} + V(q), \tag{VII.2}$$

where $p^2 := \sum_{i=1}^n (p_i)^2$. The equations (VII.1) then read $\dot{q}^i = p_i/m$ and $\dot{p}_i = -\partial V/\partial q^i$. With the force defined by $F^i := -\partial V/\partial q^i$, these are precisely Newton's equations $d^2q^i/dt^2 = F^i/m$, or $\vec{F} = m\vec{a}$. In principle, h may explicitly depend on time as well.

The equations of motion (VII.1) may or may not have a solution for all times; this depends on both h and the initial state (q,p). In the worst case, which occurs if the potential V in (VII.2) is sufficiently singular (e.g., not even Lipschitz[5]), then (VII.1) mat not even be solvable for small times. The ssituation is slightly better when (VII.1) admits a solution for given (q,p) and $|t| < \varepsilon$, for some $\varepsilon > 0$. For example, if $M = (0,1) \times \mathbb{R}$ (think of a particle moving on a finite table) and $h = p^2/2m$, then clearly the particle will roll off the table after some finite time; formally this means that (VII.1) has no solution for later times. In general, this situation applies when V is Lipschitz (cf. [8]). But ideally, one expects the equations of motion to have a solution for all $t \in \mathbb{R}$, given any initial state (q,p). In that case, the dynamics is said to be **complete**. Provided that h does *not* explicitly depend on t, it can be shown that a complete dynamics is given by an action of $\mathbb{R}$ (seen as a group in the usual, additive way) on M.

Definition VII.1 *An* **action** *of $\mathbb{R}$ on a set M is given by a map $\mathbb{R} \times S \to S$, written as $\langle t, \sigma \rangle \mapsto \sigma(t)$, satisfying $\sigma(0) = \sigma$ and $(\sigma(s))(t) = \sigma(s+t)$ for all $\sigma \in S$ and $s, t \in \mathbb{R}$. The action is called* **continuous** *or* **smooth** *when the map in question is continuous or smooth.*

It is very hard to given conditions on M and h guaranteeing that the time-evolution is given by a (continuous or smooth) action of $\mathbb{R}$ on M; this will be much easier in quantum mechanics, as we will see below. In any case, it is only in that situation that we can say that the system is deterministic. Thus the usual claim that classical mechanics is a deterministic theory (allegedly as opposed to quantum mechanics) is false!

VII.2 Quantum mechanics

Quantum mechanics is based on the postulate that the phase space is a Hilbert space H, with the additional stipulations that:

1. Only vectors of norm 1 correspond to physical states;
2. Vectors differing by a "phase", i.e., by a complex number of modulus 1, correspond to the same physical state.

In other word, $\psi \in H$ and $z\psi$ with $z \in \mathbb{C}$ and $|z| = 1$ give the same state.[6] We here stick to the physicists' convention of denoting elements of Hilbert spaces by Greek letters.[7]

[5] A function f on $\Omega \subset \mathbb{R}^n$ is called **Lipschitz** when there exists a constant $C > 0$ such that $|f(x) - f(y)| \leq C|x - y|$ for all $x, y \in \Omega$. For example, any function with bounded first derivative is Lipschitz.

[6] It follows that the true state space of a quantum-mechanical system is the **projective** Hilbert space $\mathbb{P}H$, which may be defined as the quotient $SH/\sim$, where $SH := \{f \in H \mid \|f\| = 1\}$ and $f \sim g$ iff $f = zg$ for some $z \in \mathbb{C}$ with $|z| = 1$.

[7] This notation was initially used by Schrödinger in order to make his wave mechanics, a precursor of quantum mechanics, look even more mysterious than it already was.

The reason for the first point lies in the probability interpretation of quantum mechanics. The simplest example of this interpretation is given by the quantum mechanics of a particle moving in $\mathbb{R}^3$. In that case the Hilbert space may be taken to be $H = L^2(\mathbb{R}^3)$, and Born and Pauli claimed in 1926 that the meaning of the 'wavefunction' $\psi \in L^2(\mathbb{R}^3)$ was as follows: *the probability* $P(\psi, x \in \Delta)$ *that the particle in state* ψ *is found to be in a region* $\Delta \subseteq \mathbb{R}^3$ *is*

$$P(\psi, x \in \Delta) = (\psi, \chi_\Delta \psi) = \int_\Delta d^3x \, \|\psi(x)\|^2. \tag{VII.3}$$

Here χ_Δ is the characteristic function of Δ, given by $\chi_\Delta(x) = 1$ when $x \in \Delta$ and $\chi_\Delta(x) = 0$ when $x \notin \Delta$. It follows that

$$\|\psi\|^2 = (\psi, \psi) = P(\psi, \mathbb{R}^n) = 1, \tag{VII.4}$$

since by definition of the physical system in question we assume that the particle is somewhere.

More generally, observables are represented in quantum mechanics by self-adjoint operators a on H, and one interprets the real number $(\psi, a\psi)$ as the **expectation value** of the observable a in the state ψ.[8] In the next chapter, we will associate a projection $p(\Delta)$ to each subset $\Delta \subset \sigma(a)$ of the spectrum of a. The generalization of the Born–Pauli probability interpretation of $\psi \in L^2(\mathbb{R}^3)$ to arbitrary Hilbert space is then as follows: *the probability* $P(\psi, a \in \Delta)$ *that the observable* a *takes values in* $\Delta \subset \sigma(a) \subset \mathbb{R}$ *when the system is in the state* $\psi \in H$ *is given by*

$$P(\psi, a \in \Delta) = (\psi, p(\Delta)\psi). \tag{VII.5}$$

As we shall see, $p(\sigma(a)) = 1$, so analogously to (VII.4) we may write

$$\|\psi\|^2 = (\psi, \psi) = P(\psi, p(\sigma(a))\psi) = P(\psi, a \in \sigma(a)) = 1, \tag{VII.6}$$

since in quantum mechanics one assumes a may only take values in its spectrum $\sigma(a)$, and a has to have some value. For example, $a = 1$ has $\sigma(a) = \{1\}$ and $p(1) = 1$, so that $P(\psi, 1 \in \{1\}) = (\psi, \psi) = 1$.

These considerations motivate rule 1 given at the beginning of this section; rule 2 follows from the fact that *any conceivable prediction from quantum mechanics is given by a number of the form* $(\psi, a\psi)$ *for some* $\psi \in H$ *and some self-adjoint operator* a *on* H. Thus ψ and $z\psi$ (with $|z| = 1$) yields precisely the same predictions, and therefore correspond to the same state.

VII.3 The Schrödinger equation

Quantum mechanics has a single equation of motion, known as the Schrödinger equation. The role of the Hamiltonian is now played by a certain operator h on a Hilbert space H, whose specification is part of the definition of a given physical system. The precise form of this operator is usually guessed from the form of the classical Hamiltonian. For example, if $H = L^2(\mathbb{R}^n)$ and the classical Hamiltonian is (VII.2), Schrödinger took the quantum Hamiltonian to be

$$h = -\frac{\hbar^2}{2m} \sum_{i=1}^{n} \frac{\partial^2}{\partial x_i^2} + V(x). \tag{VII.7}$$

Here $\hbar \in \mathbb{R}^+$ is a constant of nature, called **Planck's constant**, and V is seen as a multiplication operator (as the notation already suggests). It is clear that h is an unbounded operator; we shall see shortly that it has to be self-adjoint for the whole theory to make sense. In general, if a classical observable is a function $f = f(q^i, p_i)$ on $\mathbb{R}^{2n}$, then roughly speaking the 'corresponding' quantum observable is given by the operator $f(x^i, -i\hbar\partial/\partial x^i)$. This indeed yields (VII.7) from (VII.2), and even more simply says that the operator corresponding to (the i'th component of)

[8] This replaces the classical situation, where $f(\sigma)$ is simply the sharp value of an observable f in a state σ. What this really means is a matter of ongoing debate. For example, do expectation values refer to outcomes of a long series of measurements? Or to 'propensities' of the observable to have the given expectation value? Or to averages with respect to some unknown theory underlying quantum mechanics? Etcetera

position is x^i (seen as a multiplication operator), and the operator corresponding to (the i'th component of) momentum is $-i\hbar\partial/\partial x^i$. In general, however, the 'quantization' prescription

$$\begin{aligned} q^i &\mapsto x^i \\ p_i &\mapsto -i\hbar\frac{\partial}{\partial x^i} \end{aligned} \tag{VII.8}$$

is only unambiguous when f does not contain products of q's and p's.

In any case, given a quantum Hamiltonian h as an operator on some Hilbert space H, the **Schrödinger equation** reads

$$h\psi(t) = i\hbar\frac{d\psi(t)}{dt}. \tag{VII.9}$$

This equation should be seen as the quantum-mechanical analogue of Hamilton's equations (VII.1). As mentioned before, we shall establish below that h has to be self-adjoint on its domain $D(h)$; clearly eq. (VII.9) only makes sense for $\psi \in D(h)$. Nonetheless, the *solutions* of the Schrödinger equation should be defined for any $\psi \in H$, since any such ψ is allowed to be a physical state in quantum mechanics (as long as it has norm 1) and should have a well-defined time-evolution.

Let us write a solution of the Schrödinger equation with initial value ψ as

$$\psi(t) = u(t)\psi, \tag{VII.10}$$

where $u(t) : H \to H$ is some map. We assume that we are in the ideal situation that the solution is defined for all $t \in \mathbb{R}$; we shall see immediately below that this is, in fact, always the case, in constrast to the situation in classical mechanics. Indeed, if h is bounded (a situation that rarely occurs in practice except when H is finite-dimensional) and time-independent (which is true for a closed system almost by definition), one may explicitly solve (VII.9) by (VII.10) with

$$u(t) = e^{-ith/\hbar}, \tag{VII.11}$$

where the exponential is defined by its norm-convergent power-series. When h is not bounded the exponential cannot be defined in this way, but provided it is self-adjoint the exponential can be defined using the spectral theorem; see Chapter VIII. Eq. (VII.11) gives the solution of the Schrödinger equation also in that case.

VII.4 Stone's theorem

Although we have not yet established (VII.11) in the physically relevant case where h is unbounded, some desirable properties of $u(t)$ may be read off nonetheless. Taking these properties as axioms, we will then recover the notion of a Hamiltonian from Stone's theorem below. First, as in classical mechanics, when h is time-independent we expect that $(\psi(s))(t) = \psi(s+t)$, and this indeed follows from (VII.11) and the formal computation $\exp(ta)\exp(sa) = \exp((s+t)a)$, where a is any bounded operator.[9] This translates into the property

$$u(s)u(t) = u(s+t) \tag{VII.12}$$

for all $s, t \in \mathbb{R}$. Furthermore, one clearly has

$$u(0) = 0 \tag{VII.13}$$

and the strong continuity

$$\lim_{t\to 0} u(t)\psi = \psi \tag{VII.14}$$

for each $\psi \in H$; combined with (VII.12), this gives

$$\lim_{t\to s} u(t)\psi = u(s)\psi \tag{VII.15}$$

[9] The proof is the same as for the usual exponential function.

for each $s \in \mathbb{R}$. Finally, each $u(t)$ given by (VII.11) is not only linear, as is immediate from (VII.11), and in general should be the case because the Schrödinger equation is linear, but also unitary.[10] This follows from (VII.11) by a formal computation when h is bounded; in general, one could first argue that $u(t)$ has to be isometric because if ψ has norm 1, then also $\psi(t)$ should have norm 1 in order for the probability interpretation of quantum mechanics to make sense. Subsequently, (VII.12) and (VII.12) show that $u(t)$ is invertible, with inverse $u(t)^{-1} = u(-t)$. An easy exercise then shows that an invertible isometric operator is unitary.

To some up, either intuition based on the Schrödinger equation or abstract arguments show that time-evolution in quantum mechanics has the following structure. Recall Definition VII.1, in which the set M is now taken to be a Hilbert space H.

Definition VII.2 *An action of $\mathbb{R}$ on a Hilbert space H of the form $\psi(t) = u(t)\psi$, where each $u(t)$ is unitary and (VII.14) holds, is called a* **unitary representation** *of $\mathbb{R}$ on H.*[11]

Note that the properties (VII.12) and (VII.13) are implicit in the definition of an action of $\mathbb{R}$. The unitary representation as a whole, given by the map $t \mapsto u(t)$, is usually simply called u.

On this basis, the relationship between the global time-evolution and the 'infinitesimal' time-evolution given by the Schrödinger equation is completely clarified by the following result.

Theorem VII.3 *1. Let u be a unitary representation of $\mathbb{R}$ on H. Then the operator h, defined by the domain*

$$D(h) : \{f \in H \mid \lim_{t\to 0} \frac{u(t)-1}{t} f \text{ exists}\} \tag{VII.16}$$

and the action

$$hf := i \lim_{t\to 0} \frac{u(t)-1}{t} f, \tag{VII.17}$$

is self-adjoint. In particular, $D(h)$ is dense in H.

In other words, provided $\psi \in D(h)$, for each $t \in \mathbb{R}$ the vector $\psi(t) = u(t)\psi$ (which lies in $D(h)$ as well) satisfies the Schrödinger equation

$$h\psi(t) = i\frac{d\psi(t)}{dt}. \tag{VII.18}$$

2. Conversely, given a (densely defined) self-adjoint operator h on H there exists a unique unitary representation u of $\mathbb{R}$ on H that is related to h in the way just specified. Explicitly, one has

$$u(t) = e^{-ith}, \tag{VII.19}$$

where the exponential function is defined by the spectral calculus.

The last statement will be explained and proved in the next chapter. Of course, if one wants to introduce Planck's constant to recover (VII.9) and (VII.11), one should replace the operator h in this theorem by $h/\hbar$.

The first claim is proved as follows; we leave the details as an exercise. First, for any $f \in H$ and $n \in \mathbb{N}$ define

$$f_n := n \int_0^\infty ds\, e^{-ns} u(s) f.$$

Then $f_n \in D(h)$ and $f_n \to f$. Hence $D(h)$ is dense in H. Second, an easy calculation shows that h is symmetric on $D(h)$. Finally, one shows that $R(h \pm i) = H$ and invokes Theorem VI.16. ■

[10] Recall that an operator u is unitary when $uu^* = u^*u = 1$.

[11] Condition (VII.14) or (VII.15) can be shown to be equivalent to the continuity of the map $\langle t, \psi\rangle \mapsto u(t)\psi$ from $\mathbb{R} \times H$ to H. When H is separable, one can show that in the presence of (VII.12) and (VII.13), condition (VII.14) is equivalent to to the requirement that the function $t \mapsto (f, u(t)g)$ is Lebesgue measurable from $\mathbb{R}$ to $\mathbb{C}$ for each $f, g \in H$.

VII.5 States and observables

To close this chapter, we take a look at the formalism of quantum mechanics from a different perspective. Any respectable physical theory known so far has the following mathematical structure:

- One has a **state space** S; this is a **convex set** (i.e., a subset of a given vector space, such that if $\rho, \sigma \in S$ and $\lambda \in (0,1)$ then $\lambda\rho + (1-\lambda)\sigma \in S$).
- One has a **set of observables** A; this is an **ordered real vector space**: i.e., there is a so-called **positive cone** $A^+ \subset A$; this is a subset for which
  1. $a \in A^+$ and $t \in \mathbb{R}^+$ implies $ta \in A^+$;
  2. $a, b \in A^+$ implies $a + b \in A^+$;
  3. $A^+ \cap -A^+ = 0$.
- One has a **pairing** $S \times A \to \mathbb{R}$, written $\langle \omega, a \rangle \mapsto \omega(a)$, that is
  1. convex in S, i.e., $(\lambda\rho + (1-\lambda)\sigma)(a) = \lambda\rho(a) + (1-\lambda)\sigma(a)$;
  2. linear in A;
  3. **positive**, in that $\omega(a) \geq 0$ for each $a \in A^+$.

The interpretation of the pairing is that the observable a of the given system has value $\omega(a)$ in the state ω. In this sense, a state is just a value-assignment on the collection of all observables characterizing a physical system. However, it is not always clear what the 'value' of an observable denotes. To clarify this point, we make a further assumption that is satisfied in both classical and quantum mechanics, namely that the vector space of observables A has the structure of a commutative (but not necessarily associative algebra); in particular, that squares a^2 of $a \in A$ can be defined. In that case, it turns out that

$$A^+ = \{a^2 \mid a \in A\}. \tag{VII.20}$$

The **variance** of an observable a in a state ω is then defined by

$$\Delta_\omega(a) := \omega(a^2) - \omega(a)^2. \tag{VII.21}$$

We say that an observable a has a sharp value in a state ω when $\Delta_\omega(a) = 0$. In classical mechanics there exist states ω in which every observabel has a sharp value, but in quantum mechanics this is not the case due to the uncertainty principle (see below). If $\Delta_\omega(a)$ is nonzero, $\omega(a)$ is usually interpreted as the *expectation value* of a in ω. What this means in quantum mechanics is controversial; most practically minded people take it to be the average value of a with respect to a large number of measurements in which the system is prepared in the state ω each time.

Positivity of observables turns out to be an important ingredient in physical theories; think of the energy. It could be omitted from the axiomatic structure, but the notion of a state turns out to be clarified when it is included. An ordered real vector space may equivalently be characterized by a linear partial ordering $\leq$, in which $a \leq b$ implies $ta \leq tb$ for each $t \in \mathbb{R}^+$ as well as $a + c \leq b + c$ for each $c \in A$. Namely, given a positive cone one says that $a \leq b$ when $b - a \in A^+$, and vice versa, given $\leq$ one defines $A^+ := \{a \in A \mid 0 \leq a\}$. For example, if $A = C(\Omega, \mathbb{R})$, i.e., the space al all continuous functions on $\Omega \subseteq \mathbb{R}^n$, then the subspace

$$A^+ = C(\Omega, \mathbb{R}^+) \tag{VII.22}$$

of all positive functions is a positive cone in A. Of course, a positive function is the square of its square-root, so that (VII.22) coincides with (VII.20). Also, if $A = B(H)_{\mathrm{Sa}}$ is the space of all bounded self-adjoint operators on some Hilbert space H, then

$$A^+ := \{a^2 \mid a^* = a \in B(H)\} \tag{VII.23}$$

is a positive cone, which turns out to coincide with the space of all operators on H with spectrum in $\mathbb{R}^+$, which in turn coincides with the space of all self-adjoint operators a for which $(f, af) \geq 0$ for all $f \in H$.

The convex structure of the state space reflects the idea of **mixing** or incomplete knowledge: given states ρ and σ, the state $\lambda\rho + (1-\lambda)\sigma$, $\lambda \in (0,1)$ denotes the situation in which the state of the system is unknown, but is estimated to be ρ with probability λ, and σ with probability $1-\lambda$. Iterating this operation, one obtains states of the form $\omega = \sum_i P_i \omega_i$, where $P_i > 0$ and $\sum_i P_i = 1$,[12] in which one estimates that the system is in state ω_i with probability P_i. Thus the state space S can be decomposed into pure states and mixed states. A **pure state** is an element $\omega \in S$ for which $\omega = \lambda\rho + (1-\lambda)\sigma$ for $\lambda \in (0,1)$ implies $\rho = \sigma = \omega$. A **mixed state** is an element of S that is not pure; hence mixed states do allow decompositions of the sort just mentioned.

Probably the simplest nontrivial example of a convex set is $S = [0,1]$, seen as a subset of $\mathbb{R}$. The pure states in S are just 0 and 1. A more interesting example is the three-ball

$$B^3 = \{(x,y,z) \in \mathbb{R}^3 \mid x^2 + y^2 + z^2 \leq 1\}; \tag{VII.24}$$

as we shall see, this is the state space of a two-level system in quantum mechanics. Here the pure states are the points on the two-sphere

$$S^2 = \{(x,y,z) \in \mathbb{R}^3 \mid x^2 + y^2 + z^2 = 1\}. \tag{VII.25}$$

However, its is not always the case that the set of pure states in a convex set S forms the geometric boundary of S. Indeed, a triangle Δ with equal sides and equal angles is convex, but its pure states are just its corners.[13]

The physical interpretation of a pure state is that it gives the most precise characterization of the given physical system that is possible in principle. Mixed states, on the other hand, have a direct interpretation only if their decomposition into pure states is unique; this depends on the geometry of the state space. If so, mixed states have an ignornace interpretation as explained above: if $\omega = \sum_i P_i \omega_i$, where the ω_i are pure, then the system is really in one of the states ω_i. We do not know which, but we assign probability P_i to the possibility ω_i. In classical physics this is always possible. On the other hand, this interpretation often fails in quantum physics, where the decomposition of a mixed state into pure states is typically non-unique. For example, the origin in B^3 has an infinite number of possible decomopositions $0 = \omega/2 + (-\omega)/2$, where $\omega \in S^2$ is an arbitrary pure state in B^3. Indeed, it is doubtful that a quantum-mechanical system can be in a pure state at all.[14]

General considerations go as far as what has been said above; for a specific physical theory one simply has to state what the state space S, the set of observables A, as well as the pairing between the two are. In classical mechanics one starts with a phase space M, as we have seen; just think of $M = \mathbb{R}^{2n}$, as above. One then puts

$$A = C_b^\infty(S, \mathbb{R}), \tag{VII.26}$$

i.e., the set of all real-valued bounded smooth functions on M, with

$$A^+ = C_b^\infty(S, \mathbb{R}^+). \tag{VII.27}$$

Furthermore,

$$S = \mathcal{P}(M), \tag{VII.28}$$

[12] Here the sum may even be infinite provided one has a suitable topology on S.

[13] The sides of Δ do have a geometric significance in convexity theory. A **face** F of a convex set S is a convex subset of S that is closed under 'purification', in the sense that if $\omega \in F$ and $\omega = \lambda\rho + (1-\lambda)\sigma$ for some $\lambda \in (0,1)$, then $\rho \in F$ and $\sigma \in F$. Apart from Δ itself and its pure states, the faces of Δ are precisely its sides.

[14] This is due to the phenomena of entanglement and EPR-correlations.

the set of all probability measures on M. Here a **probability measure** on a topological space M is an assignment $B \mapsto P(B)$ from suitable subsets $B \subset M$ to $[0,1]$,[15] such that

$$P(\emptyset) = 0; \tag{VII.29}$$

$$P(\mathbb{R}) = 1, \tag{VII.30}$$

$$P(\cup_i B_i) = \sum_i P(B_i) \tag{VII.31}$$

for any countable collection of mutually disjoint sets B_i. Each point of $\mathbb{R}$ is interpreted as an **event**, and the number $P(B)$ associated to a subset $B \subset \mathbb{R}$ is interpreted as the probability that some event in the set B takes place. Such a measure leads to an integral

$$P(a) = \int dP(x)\, a(x) \tag{VII.32}$$

for each $a \in C^\infty(M)$, which defines the pairing between S and A. The pure states turn out to be the points x of M, seen as probability measures P_x by means of $P_x(B) = 1$ if $x \in B$ and $P_x(B) = 0$ if $x \notin B$. Consequently, one has

$$P_x(a) = a(x). \tag{VII.33}$$

In quantum mechanics the model is quite different. One starts by choosing a Hilbert space H that bears some relationship to the underlying physical system.[16] One then postulates

$$S = B_1(H)_1^+, \tag{VII.34}$$

that is, the set of positive trace-class operators on H with unit trace (cf. Section IV.3). Elements of $B_1(H)_1^+$ are called **density matrices** by physicists, and are usually denoted by ρ. Since a density matrix is compact and self-adjoint, it is of the form $\rho = \sum_i \lambda_i p_i$ by Theorem IV.2. Recall that an operator $\rho \in B(H)$ is positive when $(f, \rho f) \geq 0$ for all $f \in H$. Positivity of ρ then yields $\lambda_i \geq 0$ for all i, and $\operatorname{Tr} \rho = 1$ is equivalent to $\sum_i \lambda_i = 1$. In other words, a (bounded) operator ρ is a density matrix iff

$$\rho = \sum_i P_i p_i, \tag{VII.35}$$

where $0 < P_i \leq 1$ and $\sum_i P_i = 1$. It can be shown that the pure states are precisely the density matrices with a single term, i.e., $\rho = p$ for some one-dimensional projection p. In that case, if $p\psi = \psi$ for a unit vector ψ, physicists would simply say that the system *is* in the pure state ψ (although even this seemingly straightforward statement is denied by some). In the general case, it is very natural to interpret the numbers P_i as probabilities, so that P_i is the probability that the system is in the pure state ω_i. As already mentioned, this interpretation is actually quite problematic, as we shall now show in a very simple example.

Take $H = \mathbb{C}^2$. It can be shown (exercise) that a density matrix on $\mathbb{C}^2$ is of the form

$$\rho(x,y,z) := \frac{1}{2} \begin{pmatrix} 1+x & y+iz \\ y-iz & 1-x \end{pmatrix}, \tag{VII.36}$$

where $(x,y,z) \in \mathbb{R}^3$ satisfies $x^2 + y^2 + z^2 \leq 1$. This gives a bijection between the state space S and the three-ball B^3, which preserves the convex structure; in other words, as a convex set the state space S of a two-level system can be seen as B^3. As we have seen, the pure states form precisely the geometric boundary S^2 of B^3. Referring back to out previous example, the point zero in B^3 corresponds to the density matrix $1/2$ (times the 2×2 unit matrix). As we have seen, this density matrix admits uncountably many decompositions $1/2 \cdot 1 = 1/2(\omega_1 + \omega_2)$ into pure states ω_i: any pair of polar points on S^2 will do.

[15] These are the so-called Borel subsets of M, which are countable unions or intersections of oen or closed subsets of M.

[16] The specification of the Hilbert space plays a much weaker role in characterizing a quantum system than the specification of a phase space in characterizing a classical system. In quantum mechanics the physical interpretation of the formalism comes from the procedure of quantization, which prescribes the meaning of each operator.

Let us return to general Hilbert spaces. The collection of observables in quantum mechanics is

$$A = B(H)_{\mathrm{sa}}, \tag{VII.37}$$

the set of all bounded self-adjoint operators on H.[17] The positive cone (VII.23) can be characterized in several equivalent ways, for example, as

$$A^+ = \{a \in B(H) \mid a^* = a, \sigma(a) \subset \mathbb{R}^+\}. \tag{VII.38}$$

Finally, the pairing between states and observables is given by

$$\rho(a) := \mathrm{Tr}\, \rho a. \tag{VII.39}$$

Using (VII.35), we see that

$$\rho(a) = \sum_i P_i(\psi_i, a\psi_i), \tag{VII.40}$$

where the ψ_i are unit vectors in $p_i H$. Thus $\rho(a) \geq 0$ if $a \geq 0$, as required.

A key feature distinguishing quantum mechanics from classical mechanics is that even in pure state the variance (VII.21) is typically nonzero; in fact, one has $\Delta_\rho(a) = 0$ iff $\rho = p$ is pure and ψ (defined as above) is an eigenvector of a. The variance occurs in the famous **Heisenberg uncertainty relations**. Noting that

$$\Delta_\omega(a) = \omega((a - \omega(a))^2) \geq 0,$$

we abbreviate

$$\sigma_\omega(a) := \sqrt{\Delta_\omega(a)}. \tag{VII.41}$$

Theorem VII.4 • *Let $\rho \in B_1(H)_1^+$ be a density matrix on H, and let $a, b \in B(H)$ be self-adjoint. Then (writing $[a, b] = ab - ba$ for the commutator)*

$$\sigma_\rho(a)\sigma_\rho(b) \geq \frac{1}{2}|\rho([a, b])|. \tag{VII.42}$$

- *Let a, b be symmetric operators, and let $\psi \in D(a) \cap D(b)$ be a unit vector. Writing*

$$\sigma_\psi(a) = \sqrt{(a\psi, a\psi) - (\psi, a\psi)^2}, \tag{VII.43}$$

one has

$$\sigma_\psi(a)\sigma_\psi(b) \geq |\mathrm{Im}\,(a\psi, b\psi)|. \tag{VII.44}$$

If ψ also lies in $D(ab) \cap D(ba)$, this can be rearranged as as

$$\sigma_\psi(a)\sigma_\psi(b) \geq \frac{1}{2}|(\psi, [a, b]\psi)|. \tag{VII.45}$$

The most famous application is the case $a = q^i = x^i$ (as a multiplication operator) and $b = p_j = -i\hbar\partial/\partial x^j$ on $H = L^2(\mathbb{R}^n)$; see(VII.8). Taking $\psi \in C^\infty(\mathbb{R}^n) \cap D(x^i)$ for simplicity, with

$$D(x^i) = \{\psi \in L^2(\mathbb{R}^n) \mid \int d^n x\, (x^i)^2 |\psi(x)|^2 < \infty, \}$$

we obtain

$$\sigma_\psi(q^i)\sigma_\psi(p_j) \geq \frac{\hbar}{2}\delta^i_j. \tag{VII.46}$$

[17] Most observables are actually represented by unbounded operators. Well! Nice axiomatics requires compromises.

Chapter VIII

Spectral theory for self-adjoint operators

In this chapter we prove the spectral theorem for self-adjoint operators a. This theorem generalizes the expansion $a = \sum_i \lambda_i p_i$ of a self-adjoint compact operator (such as a hermitian matrix), or more generally of a bounded self-adjoint operator with purely discrete spectrum, in terms of its eigenvalues λ_i and the projections p_i of the corresponding eigenspaces (i.e., if $f \in p_i H$ then $af = \lambda_i f$); see Theorem IV.7. As we have pointed out before, in general a self-adjoint operator need not have any eigenvalues at all (recall the example of the multiplication operator $a(x) = \exp(-x^2)$ on $H = L^2(\mathbb{R})$), or may have mixed spectrum consisting of both eigenvalues and continuous spectrum (for example, a multiplication operator $a \in C(\Omega)$ on $L^2(\Omega)$ with compact support has eigenvalue 0 with infinite multiplicity, since any f with support disjoint from a satisfies $af = 0$, whereas the remainder of the range of a will form its continuous spectrum).[1]

It turns out that an expansion of a in terms of "infinitesimal" projections $p(t) = dE(t)$ (which become genuine projections when t is an eigenvalue, or more generally when one integrates over t) and "generalized" eigenvalues t (that is, elements of $\sigma(a)$) is always possible. Such a "spectral expansion" $a = \int dE(t)\, t$:

- Gives a complete picture of a, including its domain;
- Enables one to define functions $\varphi(a)$ of a by means of $\varphi(a) = \int dE(t)\, \varphi(t)$, where $\varphi : \mathbb{R} \to \mathbb{C}$ is an almost completely arbitrary function.[2]

In order to state the spectral theorem, we need some integration theory.

VIII.1 The Stieltjes integral

The notion of an integral, originally due to Newton, was made rigorous by Riemann in 1854. His definition was

$$\int_a^b dx\, f(x) := \lim \sum_{i=1}^{n} \Delta x_i f(\xi_i),$$

where one has made a partition of $[a, b]$ by n intervals $I_i = [x_{i-1}, x_i]$ with distinguished points $\xi_i \in [x_{i-1}, x_i]$ and size $\Delta x_i := x_i - x_{i-1}$, and the limit is over a family of such partitions in which the size Δx_i goes to zero for all i. This definition is intuitively appealing, but it has two important drawbacks: it is limited to a small class of functions that can be integrated,[3] and, even more importantly, it is tied to a specific way of assigning a "size" or "measure" Δx_i to a given interval

[1] For physicists: the spectrum of the Hamiltonian of the hydrogen atom has a mixed structure as well.

[2] Well, is has to be Borel.

[3] Consisting of the so-called Riemann-integrable functions, for which the limit exists. The class includes all continuous and all monotonous functions, but not a great deal more.

$[x_{i-1}, x_i]$. For example, one would like to be able to use a "measure" which assigns a nonzero value to a point; in the spectral theorem this will be necessary to deal with the discrete spectrum.

The modern notion of integration was introduced by Lebesgue in 1902, but we will not need this generality; for the spectral theorem it turns out to be sufficient to use the definition of integration due to Stieltjes (1894). This definition is as appealing as the one of Riemann without sharing its drawbacks, and does not nearly have the level of abstraction of Lebesgue's integral.[4]

The Stieltjes intergal (over $\mathbb{R}$) is based on the notion of a density.

Definition VIII.1 *A* **density** *is a function $\rho : \mathbb{R} \to \mathbb{R}$ that is:*

1. *monotone increasing, that is, $\rho(s) \leq \rho(t)$ if $s \leq t$;*
2. *right-continuous, that is, $\lim_{\varepsilon \to 0^+} \rho(t+\varepsilon) = \rho(t)$.*

In general, ρ need not and will not be *left*-continuous, but it follows from monotonicity that

$$\rho(t_-) := \lim_{\varepsilon \to 0^+} \rho(t-\varepsilon) \tag{VIII.1}$$

exists. For example, $\rho(t) = c$ is a density, but it turns out that the resulting integral is identically zero. Much more interesting examples are

$$\rho(t) = t, \tag{VIII.2}$$

which of course is both left- and right-continuous, and

$$\begin{aligned} \rho(t) &= 0 \ (t < 1); \\ \rho(t) &= 1 \ (t \geq 1). \end{aligned} \tag{VIII.3}$$

Now, given a density ρ, the associated Stieltjes integral $\int d\rho(t)\, f(t)$ of some function $f : \mathbb{R} \to \mathbb{C}$ is first defined for **simple** functions f. By definition, these are of the form $f = \sum_i c_i \chi_{B_i}$, where the sum is finite, $c_i \in \mathbb{R}$, $B_i \subset \mathbb{R}$ is either an *open* interval $B_i = (a, b)$ or a point $B_i = \{a\}$, all B_i are mutually disjoint, and finally χ_B is the characteristic function of B (defined by $\chi_B(t) = 1$ when $t \in B$ and $\chi_B = 0$ when $t \notin B$). For a simple function one puts

$$\int d\rho \sum_i c_i \chi_{B_i} := \sum_i c_i \int d\rho(t)\, \chi_{B_i}, \tag{VIII.4}$$

with

$$\begin{aligned} \int d\rho\, \chi_{(a,b)} &:= \rho(b_-) - \rho(a); \\ \int d\rho\, \chi_{\{a\}} &:= \rho(a) - \rho(a_-), \end{aligned} \tag{VIII.5}$$

from which it follows that

$$\int d\rho\, \chi_{[a,b]} = \rho(b) - \rho(a_-); \tag{VIII.6}$$

$$\int d\rho\, \chi_{[a,b)} = \rho(b_-) - \rho(a_-); \tag{VIII.7}$$

$$\int d\rho\, \chi_{(a,b]} = \rho(b) - \rho(a). \tag{VIII.8}$$

For an arbitrary *positive* function $\varphi : \mathbb{R} \to \mathbb{R}^+$ one then defines

$$\int d\rho(t)\, \varphi(t) \equiv \int d\rho\, \varphi := \sup_{\psi \text{ simple},\, 0 \leq \psi \leq \varphi} \left\{ \int d\rho\, \psi \right\}. \tag{VIII.9}$$

[4] Our presentation of Stieltjes integration will nevertheless borrow from Lebesgue's later work.

This supremum turns out to exist for a phenomenally large class of functions φ, namely the so-called Borel functions, and for this class the integral is *defined* by (VIII.9). If φ is bounded, it can be shown[5] that if a bounded monotone increasing sequence (φ_n) (i.e., one has

$$\varphi_0 \leq \varphi_1 \leq \cdots \varphi_n \leq \varphi_{n+1} \leq \cdots \leq c$$

pointwise) converges pointwise to φ, then

$$\int d\rho\, \varphi = \lim_{n\to\infty} \int d\rho\, \varphi_n. \tag{VIII.10}$$

In particular, one may take each φ_n to be simple, for every bounded Borel function on $\mathbb{R}$ can be approximated by such a sequence.

For arbitrary (Borel) functions $\varphi : \mathbb{R} \to \mathbb{R}$ one first decomposed $\varphi = \varphi_+ - \varphi_-$, where $\varphi_\pm \geq 0$, and defines

$$\int d\rho\, \varphi := \int d\rho\, \varphi_+ - \int d\rho\, \varphi_-. \tag{VIII.11}$$

Finally, for $\varphi : \mathbb{R} \to \mathbb{C}$ one decomposes $\varphi = \varphi' + i\varphi''$, where φ' and φ'' are real-valued, and defines $\int d\rho\, \varphi := \int d\rho\, \varphi' + i \int d\rho\, \varphi''$.

For example, for (VIII.2) one finds $\int d\rho\, \varphi = \int_{\mathbb{R}} dt\, \varphi(t)$, and for (VIII.3) one obtains $\int d\rho\, \varphi = \varphi(1)$, something quite impossible with a Riemann integral! We will often use the calculation (which is immediate from the definition):

$$\int d\rho\, \chi_{(-\infty,s]} = \int d\rho\, \chi_{(-\infty,s)} + \int d\rho\, \chi_{\{s\}} = \rho(s_-) - \rho(-\infty) + \rho(s) - \rho(s_-) = \rho(s) - \rho(-\infty). \tag{VIII.12}$$

In the next section we encounter densities ρ with the properties

$$\begin{aligned} \rho(-\infty) &= 0; \\ \rho(\infty) &= 1. \end{aligned} \tag{VIII.13}$$

We make this assumptions until the end of this section. In that case, ρ defines a probability measure on $\mathbb{R}$ (see Section VII.5) by

$$P(B) := \int d\rho\, \chi_B. \tag{VIII.14}$$

For example, the density (VIII.3) satisfies (VIII.13), and with associated probabilities $P(B) = 0$ if $1 \notin B$ and $P(B) = 1$ if $1 \in B$. In particular, $P(\{1\}) = 1$ and $P(\{a\}) = 0$ for all $a \neq 1$.

We may associate a Hilbert space $L^2(\mathbb{R}, \rho)$ with such a probability measure, whose elements are *equivalence classes* of (Borel) functions $\varphi : \mathbb{R} \to \mathbb{C}$ for which $\int d\rho(t)|\varphi(t)|^2$ is finite. It is possible that $\varphi \neq 0$ but $\|\varphi\| = 0$. To exclude this possibility, the elements of $L^2(\mathbb{R}, \rho)$ are taken to be equivalence classes $[\varphi]$, where $\varphi \sim \psi$ when $\int d\rho(t)|\varphi(t) - \psi(t)|^2 = 0$. The inner product in $L^2(\mathbb{R}, \rho)$ should strictly speaking be written as $([\varphi], [\psi]) = \int d\rho(t)\, \overline{\varphi(t)}\psi(t)$, where one should note that the right-hand side is independent of the choice of the representatives f and g in the equivalence classes $[\varphi]$ and $[\psi]$, but we usually write this simply as

$$(\varphi, \psi) := \int d\rho(t)\, \overline{\varphi(t)}\psi(t). \tag{VIII.15}$$

It can be shown that the linear span of elements of the form χ_A, $A \subset \mathbb{R}$ as specified before, (or rather the equivalence classes these define) is dense in $L^2(\mathbb{R}, \rho)$.

One should not be misled by the notation here, which falsely suggests a close analogy with $L^2(\mathbb{R}) \equiv L^2(\mathbb{R}, \mathrm{id})$. For example, the function $1_{\mathbb{R}}$ is in $L^2(\mathbb{R}, \rho)$, which is not the case for $L^2(\mathbb{R}) \equiv L^2(\mathbb{R}, \mathrm{id})$ (where $\mathrm{id}(t) = t$; cf. (VIII.2)). More spectacularly, $L^2(\mathbb{R}, \rho)$ need not even be infinite-dimensional! This completely depends on ρ. For example, with (VIII.3) one has $(\varphi, \psi) = \overline{\varphi(1)}\psi(1)$,

[5] Using the Lebesgue dominated convergence theorem

since $\int d\rho\, f = f(1)$ for any decent function f. Consequently, the map $[\varphi] \mapsto \varphi(1)$ from $L^2(\mathbb{R}, \rho)$ to $\mathbb{C}$ is isometric, and since it is clearly surjective it is unitary. Hence $L^2(\mathbb{R}, \rho) \cong \mathbb{C}$. In the next section we will encounter a density ρ for which $\int d\rho f = \sum_{i=1}^n P_i f(\lambda_i)$, where $P_i > 0$ with $\sum_i P_i = 1$ and $\lambda_i \in \mathbb{R}$. In that case, one has $L^2(\mathbb{R}, \rho) \cong \mathbb{C}^n$ via the unitary map $[\varphi] \mapsto \sqrt{P_i}\varphi(\lambda_i)e_i$, where (e_i) is the standard basis of $\mathbb{C}^n$.

VIII.2 Spectral densities

For the spectral theorem a generalization of the Stieltjes integral is needed, in which the density does not take vales in $\mathbb{R}$ but in the space of projections on a given Hilbert space H (namely the one on which the given self-adjoint operator a is defined).

Definition VIII.2 *A* **spectral density** *on a Hilbert space H is a map $E : \mathbb{R} \to B(H)$ for which each $E(t)$ is a projection (i.e., $E(t)^* = E(t)^2 = E(t)$), and:*

1. *E is monotone increasing, that is, $E(s) \leq E(t)$ if $s \leq t$ in the sense that $(f, E(s)f) \leq (f, E(t)f)$ for all $f \in H$ or (equivalently) $E(s)H \subseteq E(t)H$;*

2. *E is strongly right-continuous, that is, $\lim_{\varepsilon \to 0^+} E(t+\varepsilon)f = E(t)f$ for each $f \in H$;*

3. *$\lim_{t \to -\infty} E(t)f = 0$ and $\lim_{t \to \infty} E(t)f = f$ for each $f \in H$.*

As for ordinary densities, it follows that although E may not be left-continuous, the limit $\lim_{\varepsilon \to 0^+} E(t-\varepsilon)f$ exists for all f.

As we shall see, each self-adjoint operator a on H defines a certain spectral density. To illustrate the latter concept, we run ahead of this and mention that for a multiplication operator $a \in C(\Omega)$ on $H = L^2(\Omega)$, the associated spectral density is

$$E(t) = \chi_{a \leq t} := \chi_{\{x \in \Omega | a(x) \leq t\}}, \tag{VIII.16}$$

where $\chi_{a \leq t}$ is, of course, seen as a multiplication operator on H (note that χ_B is always a projection for any decent $B \subset \Omega$; the associated subspace $\chi_B H$ consists of all elements of L^2 with support in B). As a special case, one may take $a(x) = x$ on $H = L^2(\mathbb{R})$, in which case

$$E(t) = \chi_{(-\infty, t]}. \tag{VIII.17}$$

A completely different example is provided by the unit operator $a = 1$, which leads to

$$\begin{aligned} E(t) &= 0 \ (t < 1); \\ E(t) &= 1 \ (t \geq 1). \end{aligned} \tag{VIII.18}$$

Thirdly, if $a = \sum_{i \in I} \lambda_i p_i$, where p_i projects on the eigenvector e_i with eigenvalue λ_i and $\sum_i p_i = 1$, it turns out that

$$E(t) = \sum_{i \in I | \lambda_i \leq t} p_i. \tag{VIII.19}$$

For an arbitrary spectral density E, each $f \in H$ leads to a density ρ_f defined by

$$\rho_f(t) := (f, E(t)f), \tag{VIII.20}$$

with an associated Stieltjes integral. In addition to the two properties mentioned in Definition VIII.1, in case that $\|f\| = 1$ one evidently has

3. $\lim_{t \to -\infty} \rho_f(t) = 0$ and $\lim_{t \to \infty} \rho_f(t) = 1$;

cf. (VIII.13). In other words, if $\|f\| = 1$ then ρ_f defines a probability measure on $\mathbb{R}$.

For example, provided that $\|f\| = 1$, (VIII.18) leads to (VIII.3), with associated probabilities as specified below (VII.30), and (VIII.17) leads to $\rho_f(t) = \int_{-\infty}^{t} dx\, |f(x)|^2$. This function happens to be absolutely continuous in t (with derivative in L^1), and the rules of Stieltjes integration imply that one may then compute integrals simply by $\int d\rho(t)\, f(t) = \int_{\mathbb{R}} dt\, d\rho(t)/dt f(t)$. In the case at hand one has $d\rho_f(t)/dt = |f(t)|^2$, so that the probabilities defined by ρ_f are

$$P(B) = \int d\rho\, \chi_B = \int_{\mathbb{R}} dt\, \chi_B(t)|f(t)|^2 = \int_B dt\, |f(t)|^2. \tag{VIII.21}$$

More generally, the spectral density E in (VIII.16) defined by a multiplication operator a on $L^2(\Omega)$ leads to

$$\rho_f(t) = \int_{a \leq t} d^n x\, |f(x)|^2, \tag{VIII.22}$$

so that

$$P(B) = \int_{a^{-1}(B)} d^n x\, |f(x)|^2, \tag{VIII.23}$$

where $a^{-1}(B) = \{x \in \Omega \mid a(x) \in B\}$.

Finally, the spectral density (VIII.19) yields

$$\rho_f(t) = \sum_{i \in I | \lambda_i \leq t} P_i \tag{VIII.24}$$

in terms of

$$P_i := |(e_i, f)|^2. \tag{VIII.25}$$

These numbers are precisely the probabilities associated to ρ_f, in the sense that

$$P(B) = \sum_{i \in I | \lambda_i \in B} P_i, \tag{VIII.26}$$

so that in particular one has

$$P(\{\lambda_i\}) = |(e_i, f)|^2 \tag{VIII.27}$$

and $P(\{a\}) = 0$ if $a \neq \lambda_i$ for some $i \in I$.

The probabilities thus defined by a given spectral density on H and a unit vector $f \in H$ may be written as

$$P(B) = (f, p(B)f), \tag{VIII.28}$$

where

$$p(B) := \int dE\, \chi_B \tag{VIII.29}$$

for a subset $B \subset \mathbb{R}$ that is a finite union of points and open intervals; the definition of $\int dE\, \chi_B$ is exactly the same as (VIII.4) and (VIII.5), with ρ replaced by E. It is easily seen that each $p(B)$ is a projection, and that

1. $p(\emptyset) = 0$ and $p(\mathbb{R}) = 1$;
2. $p(A \cap B) = p(A)p(B)$;
3. $p(A \cup B) = p(A) + p(B)$ when $A \cap B = \emptyset$;
4. $p(\cup_n B_n) = \vee p(B_n)$, where $\vee p_n$ is the smallest projection p such that $p_n \leq p$ for all n.

It follows from the second item that all $p(B)$ commute among each other when B varies.

$p(B_i)p(B_j) = 0$ if $B_i \cap B_j = \emptyset$. The association $B \mapsto p(B)$ is called the **spectral measure** on $\mathbb{R}$ defined by the spectral density E; it is a projection-valed probability measure, which is of great importance for quantum mechanics.

In case that E is defined by a self-adjoint operator a, the points on $\mathbb{R}$ are interpreted as possible values a can take upon measurement, and one has the following generalization of the Born–Pauli probability interpretation of quantum mechanics:

If ψ is a unit vector in H, representing the state of the system, and a is a self-adjoint operator, representing some physical observable, then the probability that a takes some value in $B \subset \mathbb{R}$ is

$$P_\psi(a \in B) = (\psi, p(B)\psi), \tag{VIII.30}$$

where $p(B)$ is defined by (VIII.29) *in terms of the spectral density E associated to a.*

Physicists will recognize that the special cases so far agree with what they know from quantum mechanics courses; (VIII.21) is just the Pauli interpretation of the wave function, and (VIII.27) is the Born interpretation. As we shall see, ρ_f turns out to be supported by the spectrum $\sigma(a)$; this means that $P(B) = 0$ whenever $B \cap \sigma(a) = \emptyset$. Thus a self-adjoint operator can only assume values in its spectrum.

To be honest, we have only recovered the Pauli interpretation in one dimension. To do so for a particle moving in $\mathbb{R}^n$, we need to extend the probability interpretation just stated to the case of more than one spectral density. This extension was first given by von Neumann [19], as follows. Suppose one has n *commuting* self-adjoint operators a_k, with associated spectral densities E_k. It can be shown (cf. [22]) that all $E_k(t)$ commute among each other for all values of t; this is a necessary condition for the consistency of the probability interpretation. The analogue of the case of a single operator is:

The probability that in some state ψ the observables $(a_1, \ldots, a_n)$ simultaneously take some value in $B_1 \times \cdots \times B_n$ is

$$P_\psi(a_1 \in B_1, \ldots, a_n \in B_n) = (\psi, p(B_1) \cdots p(B_n)\psi), \tag{VIII.31}$$

where $p(B_i)$ is defined by (VIII.29) *with $E = E_i$, the spectral density associated to a_i.*

For example, if $H = L^2(\mathbb{R}^n)$ and $a_k = x^k$ as a multiplication operator, then $E_k(t) = \chi_{(-\infty, t_k]}$ and hence $p(B_k) = \chi_{B_k}(x^k)$ as a multiplication operator. Hence

$$P_\psi(x^1 \in B_1, \ldots, x^n \in B_n) = \int_{B_1 \times \cdots \times B_n} d^n x \, |\psi(x)|^2. \tag{VIII.32}$$

Eq. (VIII.17) is more than just a special case of a spectral density: it is to some extent the general case. To see this, given some spectral density E on a Hilbert space H we pick a vector $f \in H$ with $\|f\| = 1$, and define

$$H_f := \mathrm{span}\{E(t)f, t \in \mathbb{R}\}^-. \tag{VIII.33}$$

This is a closed subspace of H. We then define $u_f : \mathrm{span}\{E(t)f, t \in \mathbb{R}\} \to L^2(\mathbb{R}, \rho_f)$ by linear extension of

$$u_f : E(t)f \mapsto \chi_{(-\infty, t]}. \tag{VIII.34}$$

In particular, one has

$$u_f p(B) f = \chi_B; \tag{VIII.35}$$

for example, $u_f(f) = 1_{\mathbb{R}}$. An easy calculation (exercise!) shows that u_f is isometric, so that (being bounded, in particular) it can be extended to an operator $u_f : H_f \to L^2(\mathbb{R}, \rho_f)$. Furthermore, we recall that the set of all step functions is dense in $L^2(\mathbb{R}, \rho_f)$, so that $u_f(\mathrm{span}\{E(t)f, t \in \mathbb{R}\})$ is dense in $L^2(\mathbb{R}, \rho_f)$. It follows (exercise) that u_f is unitary. Now, it trivially follows from (VIII.34) that $uE(s)E(t)f = \chi_{(-\infty, s]} uE(t)f$; if $s < t$ the left-hand side is $uE(s)f = \chi_{(-\infty, s]}$, and the right-hand

side is $\chi_{(-\infty,s]}\chi_{(-\infty,t]} = \chi_{(-\infty,s]}$ as well. If $s \geq t$ one similarly finds $\chi_{(-\infty,t]} = \chi_{(-\infty,t]}$. Since u_f is unitary, and the span of all $E(t)f$ is dense in H_f by definition, one finds $u_f E(s) u_f^{-1} = \chi_{(-\infty,s]}$ as a multiplication operator on $L^2(\mathbb{R}, \rho_f)$ (whereas the right-hand side of (VIII.34) is an *element* of $L^2(\mathbb{R}, \rho_f)$). In particular, one $u_f p(B) u_f^{-1} = \chi_B$ as a multiplication operator on $L^2(\mathbb{R}, \rho_f)$ for any $B \subset \mathbb{R}$ (of the stated sort).

If $H_f = H$, we have now succeeded in showing that any spectral density is unitarily equivalent to (VIII.17), though defined on $L^2(\mathbb{R}, \rho_f)$ rather than on $L^2(\mathbb{R})$. If $H_f \neq H$, we write $f = f_1$ and pick $f_2 \in H_f^\perp$ and repeat the procedure. With H separable, we eventually arrive at $H = \oplus_n H_{f_n}$, and obtain a unitary operator

$$u = \oplus_n u_{f_n} : H \to \bigoplus_n L^2(\mathbb{R}, \rho_{f_n}) \tag{VIII.36}$$

by linear extension of $u_{f_n} : E(t) f_n \mapsto \chi_{(-\infty,t]}$, where the right-hand side is seen as an element of $L^2(\mathbb{R}, \rho_{f_n})$. As above, one obtains

$$u E(s) u^{-1} = \chi_{(-\infty,s]}, \tag{VIII.37}$$

where the right-hand side is a single multiplication operator on $\oplus_n L^2(\mathbb{R}, \rho_{f_n})$ (i.e., on any $g \in L^2(\mathbb{R}, \rho_{f_n})$ one has $uE(s)u^{-1}g = \chi_{(-\infty,s]}g$), and

$$up(B)u^{-1} = \chi_B. \tag{VIII.38}$$

Consequently, any spectral density is unitarily equivalent to (VIII.17), defined as a multiplication operator on $\oplus_n L^2(\mathbb{R}, \rho_{f_n})$.

VIII.3 Operator-valued Stieltjes integrals

Given a spectral density E on a Hilbert space H and a (Borel) function $\varphi : \mathbb{R} \to \mathbb{C}$, we are now going to define an operator

$$\varphi(E) = \int dE(t)\, \varphi(t) \tag{VIII.39}$$

on the domain

$$D_{\varphi(E)} := \{f \in H \mid \varphi \in L^2(\mathbb{R}, \rho_f) = \{f \in H \mid \int d\rho_f(t)\, |\varphi(t)|^2 < \infty\}. \tag{VIII.40}$$

The definition will be such that if $\varphi = \sum_i c_i \chi_{B_i}$ is simple, then

$$\sum_i c_i \chi_{B_i}(E) \equiv \int dE \sum_i c_i \chi_{B_i} = \sum_i c_i p(B_i), \tag{VIII.41}$$

where $p(B)$ was defined in (VIII.29). Note, in any case, that it is a highly nontrivial fact (exercise) that $D_{\varphi(E)}$ is a dense linear subspace of H.

For any bounded function φ one has $\varphi \in L^2(\mathbb{R}, \rho_f)$ for all $f \in H$ by (VII.30), so $D_{\varphi(E)} = H$, hence one expects $\varphi(E)$ to be a bounded operator. Indeed, when φ is simple (and hence bounded) the same calculation that establishes the unitarity of the map u_f in the previous section yields

$$\|\varphi(E)f\| = \|\varphi\|_{L^2(\mathbb{R},\rho_f)}. \tag{VIII.42}$$

Since

$$\|\varphi\|^2_{L^2(\mathbb{R},\rho_f)} = \int d\rho_f\, |\varphi(t)|^2 \leq \|\varphi\|^2_\infty (\rho_f(\infty) - \rho_f(-\infty)) = \|\varphi\|^2_\infty,$$

we see that $\varphi(E)$ is bounded for simple φ. We now first define $\varphi(E)$ for a bounded function φ, and will find the same conclusion.

Suppose that $\varphi \geq 0$ and let (φ_n) be a bounded monotone increasing sequence (φ_n) of simple functions converging pointwise to φ; cf. (VIII.10) and surrounding text. Such a sequence exists by a deep fact of real analysis. Inspired by (VIII.10), we put

$$\varphi(E)f := \lim_n \varphi_n(E)f \tag{VIII.43}$$

for each $f \in H$, where $\varphi_n(E)$ is defined by linearity and (VIII.29), that is,

$$\sum_k c_k \chi_{B_k}(E) = \sum_k c_k p(B_k), \tag{VIII.44}$$

where $p(B)$ is given in (VIII.29).

To see that this definition makes sense, we introduce and important proposition, whose proof we leave as an exercise. Notationwise, if a and b are bounded self-adjoint operators, $a \leq b$ by definition means that $(f, af) \leq (f, bf)$ for all $f \in H$

Proposition VIII.3 *Each bounded sequence (a_n) of monotone increasing bounded self-adjoint operators (i.e., one has*

$$a_0 \leq a_1 \leq \cdots a_n \leq a_{n+1} \leq \cdots \leq c1 \tag{VIII.45}$$

for some constant c; equivalently, $\|a_n\| \leq c$ for all n) converges strongly (that is, in the sense that $(a_n f)$ converges in H for each $f \in H$) to a bounded self-adjoint operator a, which is the least upper bound of the given sequence (i.e., $a_n \leq a$ for all n, and if $a_n \leq b$ for all n then $a \leq b$).

This proposition should be compared with the analogous result for real numbers, which is indeed a key step in its proof. Now, it is easy to show (exercise), yet of great importance, that:

Lemma VIII.4 *If (φ_n) is a monotone increasing sequence (φ_n) of simple functions bounded by c, then the sequence of operators $(a_n := \varphi_n(E))$ satisfies* (VIII.45) *for the same value of c.*

Consequently, (VIII.43) makes good sense by virtue of Proposition VIII.3. In particular, $\varphi(E)$ is bounded for bounded φ, as expected. For general φ, we then define the integral $\varphi(E)$ by decomposing φ into two (in the real case) of four (in the complex case) positive parts, as in the definition of the ordinary Stieltjes integral.

To define $\varphi(E)$ for arbitrary, i.e., not necessarily bounded (Borel) functions, we need a slighty more subtle procedure. We once again use the fact that the collection of simple functions is dense in $L^2(\mathbb{R}, \rho_f)$ for each E and each $f \in H$. If now $\varphi \in L^2(\mathbb{R}, \rho_f)$, so that $f \in D_{\varphi(E)}$ (see (VIII.40)), we pick a sequence of simple functions φ_n converging to φ in $L^2(\mathbb{R}, \rho_f)$, and define $\varphi(E)$ by (VIII.43) once more. To see that this limit exists, we note that (φ_n) is a Cauchy sequence in $L^2(\mathbb{R}, \rho_f)$, so that $(\varphi_n(E)f)$ is a Cauchy sequence in H, since

$$\|\varphi_n(E)f - \varphi_m(E)f\|_H = \|\varphi_n - \varphi_m\|_{L^2(\mathbb{R}, \rho_f)}.$$

In this limiting procedure one may well lose the boundedness of $\varphi(E)$ for simple φ.[6] Nonetheless, from (VIII.42) (established for simple functions φ) and the definition of $\varphi(E)$ one concludes that (VIII.42) holds for arbitrary (Borel) functions φ, as long as $f \in D_{\varphi(E)}$, so that the right-hand side (and consequently the left-hand side) is finite. Moreover, one has a very simple criterion for self-adjointness:

Proposition VIII.5 *The operator $\varphi(E)$ defined by* (VIII.39) *and* (VIII.40) *has adjoint*

$$\varphi(E)^* = \overline{\varphi}(E), \tag{VIII.46}$$

where $\overline{\varphi}$ is the complex conjugate of φ. In particular, $\varphi(E)$ is self-adjoint when φ is real-valued.

[6] If φ is bounded, the two definitions we have given of $\varphi(E)$ are consistent, since by the Lebesgue dominated convergence theorem one has $\varphi_n \to \varphi$ in $L^2(\mathbb{R}, \rho_f)$ for all $f \in H$. Hence the second definition includes the first, and in fact enables one to compute $\varphi(E)$ using a larger class of approximants that the first definition.

We leave the proof as an exercise.

An equivalent way to define $\varphi(E)$ for general φ is to regard φ as a (possibly unbounded) multiplication operator on $\bigoplus_n L^2(\mathbb{R}, \rho_{f_n})$, and then put

$$\varphi(E) = u^{-1}\varphi u, \tag{VIII.47}$$

where u was defined around (VIII.36); cf. (VIII.38). To be precise, let φ_n be φ as a multiplication operator on $H_n = L^2(\mathbb{R}, \rho_{f_n})$ (where $f_n \in D_{\varphi(E)}$), which is defined and self-adjoint on

$$D(\varphi_n) = \{\psi \in L^2(\mathbb{R}, \rho_{f_n}) \mid \varphi\psi \in L^2(\mathbb{R}, \rho_{f_n})\}. \tag{VIII.48}$$

We then use the following result (exercise):

Proposition VIII.6 *Let $H = \bigoplus_n H_n$ and suppose that for each n one has a self-adjoint operator a_n on H_n. Then there is a unique self-adjoint operator a on H whose restriction to H_n is a_n, namely the operator defined on the domain*

$$D(a) = \{f = \sum_n f_n \mid f_n \in D(a_n) \,\&\, \sum_n \|a_n f_n\|^2 < \infty\} \tag{VIII.49}$$

by $a\sum_n f_n := \sum_n a_n f_n$.

This makes it clear what the domain of the multiplication operator φ on $\bigoplus_n L^2(\mathbb{R}, \rho_{f_n})$, and hence provides a complete interpretation of (VIII.47).

VIII.4 The spectral theorem for bounded operators

The central result of this chapter is Theorem VIII.12 in the next section, but for pedagogical reasons we first state and prove the bounded case (to which the proof of the general case will even be reduced![7]).

Theorem VIII.7 *Let a be a bounded self-adjoint operator on H. Then there exists a unique spectral density E with the property*

$$a = \mathrm{id}(E) = \int dE(t)\, t. \tag{VIII.50}$$

We first construct the $E(t)$ from a. To do so, we are going to define a self-adjoint operator $\varphi(a)$ for each bounded real-valued (Borel) function φ on $\mathbb{R}$. This procedure will be analogous to the definition of $\varphi(E)$: the definition will first be given for a class of functions φ_n for which it is a priori clear what $\varphi_n(a)$ should mean, and the general case will be handled by approximating an arbitrary φ by a pointwise convergent monotone sequence of the φ_n in the given clas. The difference between the construction of $\varphi(E)$ and that of $\varphi(a)$ is that in the former case the φ_n are simple functions, whereas in the latter case they are polynomials.

So let a be a bounded self-adjoint operator on H. For a polynomial $p(t) = \sum_k c_k t^k$ it is clear that $p(a)$ should equal

$$p(a) = \sum_k c_k a^k. \tag{VIII.51}$$

This is again a bounded operator by (III.4), which is self-adjoint if $c_k \in \mathbb{R}$. In particular,

$$\mathrm{id}(a) = a, \tag{VIII.52}$$

where $\mathrm{id}(t) = t$. Note that $p(a)$ is a bounded operator despite the fact that p is generally unbounded as a function on R. The reason for this is that a satisfies a bound $\alpha_1 1 \leq a \leq a_2 1$, where $\alpha_i \in \mathbb{R}$; it follows from the Cauchy–Schwarz inequality that this is certainly the case for $\alpha_1 = -\|a\|$ and

[7] For a uniform but somehwat elaborate proof for the bounded and unbounded case at one stroke see [26]. Our proof combines ideas from [24] and [20].

$\alpha_2 = \|a\|$, but we may take $\alpha_1 = \inf\{(f, af), \|f\| = 1\}$ and $\alpha_2 = \sup\{(f, af), \|f\| = 1\}$ (one of these will equal $\pm\|a\|$). We write $I_a := [\alpha_1, \alpha_2]$. It turns out that in defining $\varphi(a)$ only the values of φ on I_a are relevant, so that we may regard φ as a function from I_a to $\mathbb{R}$. Clearly, any polynomial (or, more generally, any continuous function) is bounded on I_a.

It is of central importance for what follows that the analogue of Lemma VIII.4 holds:

Lemma VIII.8 *If (φ_n) is a monotone increasing sequence (φ_n) of real polynomials on I_a bounded by c, then the sequence of operators $(a_n := \varphi_n(a))$ satisfies* (VIII.45) *for the same value of c.*

Once again, we leave the proof of this lemma as an exercise. It shows, for example, that one cannot restrict the polynomials p to an interval smaller than I_a, for if $p(t) \leq q(t)$ merely on such a smaller interval, then one may not necessarily have $p(a) \leq q(a)$.

Similarly, one has

Lemma VIII.9 *If pq is the pointwise product of two polynomials p and q, then $(pq)(a) = p(a)q(a)$, and similarly for $p + q$ and cp, $c \in \mathbb{R}$. Moreover, one has $p(a)^* = \overline{p}(a)$ (where $\overline{p}$ is the complex conjugate of p). Finally, one has*

$$\|p(a)\| \leq \|p\|_\infty = \sup_{t \in I_a} |p(t)|. \tag{VIII.53}$$

Now let $\varphi : I_a \to \mathbb{R}^+$ be a bounded positive (Borel) function. It is a deep fact of analysis (see, e.g., [20]) that there exists a bounded monotone increasing sequence (φ_n) of polynomials on I_a that converges pointwise to φ. Consequently, Proposition VIII.3 enables us to define

$$\varphi(a)f := \lim_n \varphi_n(a)f \tag{VIII.54}$$

for each $f \in H$, where $\varphi_n(a)$ is defined by (VIII.51). For arbitrary (Borel) $\varphi : I_a \to \mathbb{C}$, one then defines $\varphi(a)$ by decomposing φ as a sum of four positive parts.

Thus, for a given bounded self-adjoint operator a, we have defined an operator $\varphi(a)$ for each bounded Borel function $\varphi : I_a \to \mathbb{C}$, which is is self-adjoint if φ is real-valued. For fixed a the correspondence $a \mapsto \varphi(a)$ may also be reagrded as a map $\varphi \mapsto \varphi(a)$ from the space $\mathcal{B}_b(I_a)$ of bounded Borel functions on I_a to $B(H)$ (where H is the Hilbert space on which a is defined). This map preserves all good properties of its restriction to polynomials. To state these, note that $\mathcal{B}_b(I_a)$ is an algebra under pointwise operations. In particular, one has

Proposition VIII.10 *Let a be a bounded self-adjoint operator on H, with I_a as above.*

1. *The map $\varphi \mapsto \varphi(a)$ from the space $\mathcal{B}_b(I_a)$ of bounded (Borel) functions on I_a to $B(H)$ is an algebra homomorphism, which in addition satisfies $\varphi(a)^* = \overline{\varphi}(a)$.*
2. *If (φ_n) is a bounded monotone sequence of (Borel) functions on I_a converging pointwise to φ, then $\varphi(a) = \lim_n \varphi_n(a)$ (strong limit, i.e., $\varphi(a)f = \lim_n \varphi_n(a)f$ for each $f \in H$).*
3. *One has*
$$\|\varphi(a)\| \leq \|\varphi\|_\infty. \tag{VIII.55}$$

This proposition is sort of obvious given Lemmas VIII.8 and VIII.9 along with the definition of $\varphi(a)$ by (VIII.54); we refer to [20] (Thm. 4.5.4) for a proof.

After this preparation, we define $E(t)$ in terms of a by

$$\begin{aligned} E(t) &= 0 \quad (t < \alpha_1); \\ E(t) &= \chi_{[\alpha_1,t]}(a) \quad (t \in [\alpha_1, \alpha_2]); \\ E(t) &= 1 \quad (t > \alpha_2). \end{aligned} \tag{VIII.56}$$

Using Proposition VIII.10, it is easily shown that E satisfies the axioms of a spectral density. For example, each $E(t)$ is a projection because (for $t \in [\alpha_1, \alpha_2]$)

$$E(t)^2 = \chi_{[\alpha_1,t]}(a)^2 = \chi^2_{[\alpha_1,t]}(a) = \chi_{[\alpha_1,t]}(a) = E(t).$$

Furthermore, since $\chi_{[\alpha_1,t]}$ is right-continuous as a function of x, the right-continuity of $E(t)$ follows from the second part of the proposition.

Recall (VIII.29), and notice that

$$p(B) = \chi_B(a) \tag{VIII.57}$$

for $B \subset \mathbb{R}$ (restricted as before) by (VIII.44) and (VIII.56). Here $\chi_B(a) := \chi_{B\cap I_a}(a)$, since $\chi_B(a)$ is not defined as such.[8] For example, for $x, y \in I_a$ one has

$$\chi_{(x,y]}(E) = E(y) - E(x) = \chi_{[\alpha_1,y]}(a) - \chi_{[\alpha_1,x]}(a) = (\chi_{[\alpha_1,y]} - \chi_{[\alpha_1,x]})(a) = \chi_{(x,y]}(a).$$

The preceding calculation shows that

$$\varphi_n(E) = \varphi_n(a) \tag{VIII.58}$$

for all simple functions φ_n. Hence if $\varphi_n \to \varphi$ in the stated way (i.e., pointwise and monotone increasing), then (VIII.58), (VIII.43), and Proposition VIII.10.2 yield

$$\varphi(E) = \lim_n \varphi_n(E) = \lim_n \varphi_n(a) = \varphi(a),$$

where both limits are strong. In other words (cf. (VIII.39)),

$$\varphi(E) = \varphi(a). \tag{VIII.59}$$

Clearly, (VIII.50) follows as a special case.

The uniqueness of E may be derived from **Stone's formula**:

$$\rho_f(t) = \lim_{\delta\to 0^+} \lim_{\varepsilon\to 0^+} \int_{-\infty}^{t+\delta} \frac{dx}{2\pi i}\, (f, [(a - x - i\varepsilon)^{-1} - (a - x + i\varepsilon)^{-1}]f), \tag{VIII.60}$$

which determines ρ_f and hence E (cf. (VIII.20))[9] in terms of a, given (VIII.59). Stone's formula follows from Stieltjes' formula

$$\rho(t) = \lim_{\delta\to 0^+} \lim_{\varepsilon\to 0^+} \int_{-\infty}^{t+\delta} \frac{dx}{2\pi i}\, [g(x + i\varepsilon) - g(x - i\varepsilon)], \tag{VIII.61}$$

where, for $z \in \mathbb{C}\backslash\mathbb{R}$,

$$g(z) := \int_{-\infty}^{\infty} d\rho(t)\, \frac{1}{t - z}. \tag{VIII.62}$$

Namely, putting $\varphi : t \mapsto (t - z)^{-1}$ in VIII.59 one finds

$$\frac{1}{a - z} = \int dE(t)\, \frac{1}{t - z} \tag{VIII.63}$$

and hence, for $\rho = \rho_f$,

$$g(z) = (f, (a - z)^{-1} f). \tag{VIII.64}$$

Eq. (VIII.61) then immediately yields (VIII.60).[10]

This finishes the proof of Theorem VIII.7. ∎

The spectral theorem is of fundamental importance to quantum mechanics, where the spectral density E defined by a, rather than a itself determines the probability interpretation of the theory; see (VIII.30) and (VIII.31). More generally, E is important because it contains all spectral information about a. We state the result also for unbounded operators, as we will see in the next section that the proof below (for the bounded case) also implies the result in general.

[8] It is possible to define E by (VIII.57), because p determines E just as well as E determines p.

[9] If b is any bounded self-adjoint operator, then $(f, bf) = 0$ for all $f \in H$ implies $b = 0$. Hence b is determined by the collection of all (f, bf).

[10] Stone's formula may be used to *define* E in terms of a, see [26], but although this leads to a unified proof of the spectral theorem for bounded and unbounded operators, it gives little insight in the matter.

Theorem VIII.11 *Let a be a self-adjoint operator, with associated spectral density E (see* (VIII.56)*) and projection-valued measure p (cf.* (VIII.57) *and* (VIII.29)*).*

1. *One has $\lambda \in \sigma(a)$ iff $p(\lambda-\epsilon,\lambda+\epsilon) \neq 0$ for all $\epsilon > 0$.*
2. *One has $\lambda \in \sigma_d(a)$ iff $p(\{\lambda\}) \neq 0$, in which case $p(\{\lambda\})$ equals the projection onto the eigenspace H_λ of a.*[11]

The implication "$\Rightarrow$" in part 1 is logically equivalent to: if $p(\lambda-\epsilon,\lambda+\epsilon)=0$ for some $\epsilon>0$, then $\lambda \in \rho(a)$, i.e., $(a-\lambda)^{-1}$ exists (as a bounded operator). Indeed, define

$$\begin{aligned} \alpha_\lambda(t) &= \frac{1}{t-\lambda};\ t \notin (\lambda-\epsilon,\lambda+\epsilon); \\ \alpha_\lambda(t) &= 0;\ t \in (\lambda-\epsilon,\lambda+\epsilon) \end{aligned}$$

Then $\|\alpha_\lambda\|_\infty \leq \epsilon$ and

$$\alpha_\lambda(\mathrm{id}-\lambda) = (\mathrm{id}-\lambda)\alpha_\lambda = 1 \tag{VIII.65}$$

on $\mathbb{R}\backslash(\lambda-\epsilon,\lambda+\epsilon)$. Now, if $p(\lambda-\epsilon,\lambda+\epsilon)=0$, then the definition of the operator-valued Stieltjes integral implies that

$$\int dE\,\psi = \int dE\,\chi_{\mathbb{R}\backslash(\lambda-\epsilon,\lambda+\epsilon)}\psi \tag{VIII.66}$$

for all reasonable (e.g., bounded Borel) functions ψ. By (VIII.59) for $\varphi = \alpha_\lambda(\mathrm{id}-\lambda)$ (and similarly for $\varphi = (\mathrm{id}-\lambda)\alpha_\lambda$) one has

$$(\alpha_\lambda(\mathrm{id}-\lambda))(a) = \int dE(t)\,\alpha_\lambda(t)(t-\lambda) = 1 \tag{VIII.67}$$

by (VIII.66) and (VIII.65). By Proposition VIII.10.1 the left-hand side equals $\alpha_\lambda(a)(a-\lambda)$, hence $\alpha_\lambda(a)(a-\lambda)=1$, and similarly $(a-\lambda)\alpha_\lambda(a)=1$. Hence $\alpha_\lambda(a)=(a-\lambda)^{-1}$, so that $\lambda \in \rho(a)$.

In the "$\Leftarrow$" direction, take $\epsilon = 1/n$ and pick some $f_n \in p(\lambda-1/n,\lambda+1/n)H$ with norm 1; such f exists by assumption. Then, using by Proposition VIII.10.3 and (VIII.57),

$$\|(a-\lambda)f_n\| = \|(a-\lambda)p(\lambda-1/n,\lambda+1/n)f_n\| \leq \|(a-\lambda)p(\lambda-1/n,\lambda+1/n)\| \leq \|(\mathrm{id}-\lambda)\chi_{(\lambda-1/n,\lambda+1/n)}\|_\infty.$$

The right-hand side is $\leq 1/n$, hence $\|(a-\lambda)f_n\| \to 0$. By Theorem VI.18, $\lambda \in \sigma(a)$.

To prove part 2, we write $p(\lambda) \equiv p(\{\lambda\})$ and denote the projection onto the eigenspace H_λ by p_λ (provided $\lambda \in \sigma_d(a)$). We have $p(\lambda) = \chi_\lambda(a)$ by (VIII.29); we write $\chi_\lambda \equiv \chi_{\{\lambda\}}$. Hence

$$ap(\lambda) = \mathrm{id}(a)\chi_\lambda(a) = (\mathrm{id}\chi_\lambda)(a) = (\lambda 1\chi_\lambda)(a) = \lambda 1(a)\chi_\lambda)(a) = \lambda p(\lambda).$$

Consequently, if $p(\lambda) \neq 0$ then $p_\lambda \neq 0$, so that $\lambda \in \sigma_d(a)$, and

$$p(\lambda) \leq p_\lambda, \tag{VIII.68}$$

since $p(\lambda)H \subseteq p_\lambda H = H_\lambda$, as we have just shown.

Conversely, let $\varphi_n(t) := (\inf\{1,|\lambda-t|\})^{1/n}$, so that $\varphi_n \to \chi_{\mathbb{R}\backslash\{\lambda\}}$ pointwise. Hence by Proposition VIII.10.2 one has $\varphi_n(a) \to \chi_{\mathbb{R}\backslash\{\lambda\}}(a) = p(\mathbb{R}\backslash\{\lambda\})$. Now, if $\lambda \in \sigma_d(a)$, so that $p_\lambda \neq 0$, then

$$\varphi_n(a)p_\lambda f = \varphi_n(\lambda)p_\lambda f = 0 \tag{VIII.69}$$

for all $f \in H$; for in general one has $\varphi(a)p_\lambda f = \varphi(\lambda)p_\lambda$, as can be seen by approximating φ by polynomials (for which the property is clearly true) and using Proposition VIII.10.2. Letting $n \to \infty$ in (VIII.69) yields $p(\mathbb{R}\backslash\{\lambda\})p_\lambda = 0$, or $p(\lambda)p_\lambda = p_\lambda$, as $p(\mathbb{R}\backslash\{\lambda\}) + p(\lambda) = 1$. In other words,

$$p(\lambda) \geq p_\lambda. \tag{VIII.70}$$

With (VIII.68), we obtain $p(\lambda) = p_\lambda$. ■

[11] Recall that the discrete spectrum $\sigma_d(a)$ consists of all eigenvalues of a.

As a corollary, it follows that if $\sigma(a) = \sigma_d(a) = \{\lambda_i\}_{\imath\in I}$, then $\int dE\,\varphi = \sum_{\imath\in I}\varphi(i)$, and consequently

$$a = \int dE\,\mathrm{id} = \sum_{\imath\in I}\lambda_i p(\lambda). \tag{VIII.71}$$

As we have seen, this applies in particular to compact operators, but the class of operators with purely discrete spectrum is considerably larger (e.g. $a = 1$ is not compact when H is infinite-dimensional, yet has $\sigma(a) = \sigma_d(a) = \{1\}$).

VIII.5 The spectral theorem for unbounded operators

Formally, the statement of the spectral theorem for possibly unbounded operators is the same as in the bounded case (cf. Theorem VIII.7):

Theorem VIII.12 *Let a be a self-adjoint operator on H. Then there exists a unique spectral density E on H with the property*

$$a = \int dE(t)\,t. \tag{VIII.72}$$

Let us note, however, that this equality entails more than in the bounded case, since the definition of an operator includes the specification of its domain. By definition, the domain of the right-hand side is given by (VIII.40) with $\varphi = \mathrm{id}$; hence Theorem VIII.7 *includes* the claim that

$$D(a) = \{f \in H \mid \int d\rho_f(t)\,t^2 < \infty\}. \tag{VIII.73}$$

We are going to prove Theorem VIII.12 using a method due to von Neumann [19], which derives the spectral theorem for unbounded self-adjoint operators from the spectral theorem for unitary operators:

Theorem VIII.13 *Let u be a unitary operator on H. Then there exists a unique spectral density E on H with the properties $E(0) = 0$ (hence $E(t) = 0$ for all $t \le 0$), $E(2\pi) = 1$ (hence $E(t) = 1$ for all $t \ge 2\pi$), and*

$$u = \int_0^{2\pi} dE(t)\,e^{it}. \tag{VIII.74}$$

The proof is practically the same as for self-adjoint operators, with the following difference. In the self-adjoint case we started with polynomials p in a real variable t, defined $p(a)$ in the obvious way, and subsequently defined $\varphi(a)$ for arbitrary bounded (Borel) functions φ by approximating the latter by polynomials. The properties $p(a)^* = \overline{p}(a)$ and $p(a) \le q(a)$ if $p(t) \le q(t)$ for all (relevant) t then implied the corresponding properties for arbitrary φ (see Proposition VIII.10). These properties hold by virtue of the equality $a^* = a$. Now, for unitary operators u one instead has

$$u^*u = uu^* = 1. \tag{VIII.75}$$

Reflecting this change, we now start from polynomials in the variable $\exp(it)$, so that the map $\varphi \mapsto \varphi(u)$ is initially defined for functions of the form $\varphi(t) = \sum_k c_k \exp(itk)$, which is mapped to $\varphi_e(u) := \sum_k c_k u^k$ (whereas for self-adjoint a this φ would be mapped into $\varphi(a) = \sum_k c_k \exp(ika)$). Hence we may assume that $0 < t \le 2\pi$. In particular, writing

$$e(t) := \exp(it), \tag{VIII.76}$$

one has

$$e \mapsto e_e(u) = u. \tag{VIII.77}$$

Clearly, (VIII.75) is reflected by the identity $\overline{e}e = e\overline{e} = 1$, but also more generally one has $\varphi_e(u)^* = \overline{\varphi}_e(u)$ and $\varphi_e(u) \le \psi_e(u)$ if $\varphi(t) \le \psi(t)$ for all $t \in (0, 2\pi]$ for functions φ, ψ of the said form; Proposition VIII.10 holds with a replaced by u and φ replaced by φ_e.

From this point onwards, the proof of the spectral theorem is the same as in the self-adjoint case. Any positive bounded Borel function on the interval $(0, 2\pi]$ can be approximated pointwise by a monotone increasing sequence of polynomials in $\exp(it)$, just as it can be thus approximated by plynomials in t (as we did in the self-adjoint case).[12] Proposition VIII.10 holds with a replaced by u and I_a replaced by $(0, 2\pi]$. As in (VIII.56), we define the spectral density E by

$$\begin{aligned} E(t) &= 0 \quad (t \leq 0); \\ E(t) &= (\chi_{(0,t]})_e(u) \quad (t \in (0, 2\pi]); \\ E(t) &= 1 \quad (t > 2\pi). \end{aligned} \tag{VIII.78}$$

This guarantees the property $p(B) = (\chi_B)_e(u)$ (cf. (VIII.57)), from which $\varphi(E) = \varphi_e(u)$ for simple functions φ. Approximating a general bounded Borel function φ by simple functions φ_n as in the self-adjoint case, the numerical convergence $\varphi_n \to \varphi$ (pointwise) implies the (strong) operator convergence $\varphi_n(E) \to \varphi(E)$ and $(\varphi_n)_e(u) \to \varphi_e(u)$. Since $\varphi_n(E) = (\varphi_n)_e(u)$, this gives

$$\varphi(E) = \varphi_e(u). \tag{VIII.79}$$

Taking $\varphi = e$ and using (VIII.76) and (VIII.77)(as well as the notation (VIII.39)), we obtain (VIII.74). ■

To prove Theorem VIII.12 from Theorem VIII.13, von Neumann introduced an operator version of the **Cayley transform**. For numbers, this is a map $\kappa : \mathbb{R} \to \mathbb{C}$ defined by

$$\kappa(t) := \frac{t - i}{t + i}. \tag{VIII.80}$$

This maps $\mathbb{R}$ homeomorphically (that is, continuously and bijectively with continuous inverse) to $\mathbb{T}\backslash\{1\}$ (i.e., the unit circle in the complex plane minus the point 1). Moreover, since formally $\kappa(-\infty) = \kappa(\infty) = 1$, it maps the one-point compactification $\dot{\mathbb{R}}$ homeomorphically to $\mathbb{T}$. The inverse is

$$\kappa^{-1}(z) = i\frac{1 + z}{1 - z}, \tag{VIII.81}$$

where $z \in \mathbb{T}\backslash\{1\}$. Now let a be a self-adjoint operator. We see from Theorem VI.16 that $-i \in \rho(a)$, so that $a + i : D(a) \to H$ is a bijection with bounded inverse $(a + i)^{-1} : H \to D(a)$. Composing with $a - i : D(a) \to H$, which is a bijection, too, we see that

$$\kappa(a) := \frac{a - i}{a + i} = (a - i)(a + i)^{-1} \tag{VIII.82}$$

is a bijection from H to H. In a diagram, we have

$$H \overset{(a+i)^{-1}}{\longrightarrow} D(a) \overset{a-i}{\longrightarrow} H.$$

Furthermore, since $a^* = a$ one computes $\|(a + i)f\| = \|(a - i)f\|$ for all $f \in D(a)$, and putting $f = (a + i)^{-1}g$ we find $\|g\| = \|\kappa(a)\|$. In other words, $\kappa(a)$ is an isometry, and since an invertible isometry is unitary, we conclude that $\kappa(a)$ *is unitary*. We note that

$$R(1 - \kappa(a)) = D(a), \tag{VIII.83}$$

since $1 - \kappa(a) = 2i(a + i)^{-1}$, and as we have seen $(a + i)^{-1} : H \to D(a)$ is a bijection.

Conversely, let u be a unitary operator with $R(1 - u)^- = H$. (For example, $u = 1$ does *not* satisfy this assumption!) It is an easy exercise to show that this implies that $1 - u$ is injective, so that $1 - u : H \to R(1 - u)$ is invertible. We may then define an operator on the dense domain $D(\kappa^{-1}(u)) := R(1 - u)$ by

$$\kappa^{-1}(u) := i\frac{1 + u}{1 - u} = i(1 + u)(1 - u)^{-1}. \tag{VIII.84}$$

[12] This is a property of Fourier series that we will not prove in this notes.

If $u = \kappa(a)$ then clearly $\kappa^{-1}(u) = a$ (including its domain), justifying the notation κ^{-1}. More generally, one can show (cf. the next section) that $\kappa^{-1}(u)$ is self-adjoint; this is not needed for the present section. Consequently:

Proposition VIII.14 *The operator Cayley transform $a \mapsto \kappa(a)$ establishes a bijection between the class of self-adjoint operators a and the class of unitary operators u with $R(1-u)^- = H$. This bijection preserves the spectrum in the sense that*

$$\sigma(\kappa(a)) = \kappa(\sigma(a)); \tag{VIII.85}$$

$$\sigma_d(\kappa(a)) = \kappa(\sigma_d(a)). \tag{VIII.86}$$

We leave the proof of the second part to the reader; it implies that Theorem VIII.11 holds for unbounded operators as well.

Now let $u = \kappa(a)$ and put

$$\varphi(t) = \kappa^{-1}(\exp(it)) \tag{VIII.87}$$

in (VIII.79); this yields $\varphi_e(u) = \kappa^{-1}(u) = a$, so that

$$a = i \int_0^{2\pi} dE(t)\, \frac{1+e^{it}}{1-e^{it}}. \tag{VIII.88}$$

A chnage of variables $t \mapsto \lambda$, where $\lambda(t) := \kappa^{-1}(\exp(it))$ gives

$$a = \int_{\mathbb{R}} d\tilde{E}(\lambda)\, \lambda, \tag{VIII.89}$$

where $\tilde{E}(\lambda) := E(t(\lambda))$, where $t(\lambda)$ is the unique $t \in (0, 2\pi]$ for which $\kappa(\lambda) = \exp(it)$. With a change of notation, this is precisely (VIII.72), up to the domain. According to (VIII.40), the domain of the right-hand side of (VIII.88) is

$$D_{\varphi(E)} = \left\{ f \in H \mid \int_0^{2\pi} d(f, E(t)f) \left| \frac{1+e^{it}}{1-e^{it}} \right|^2 < \infty \right\}. \tag{VIII.90}$$

If $f \in R(1-u)$, so that $f = (1-u)g$ for some $g \in H$, then, using (VIII.42) with φ given by (VIII.87),

$$\|\varphi\|_{L^2((0,2\pi],\rho_f)} = \|\varphi(E)f\| = \|(1+u)g\| < \infty,$$

since $(1-u)\varphi(E) = (1+u)$ by Proposition VIII.10 (for u), while $(1+u)$ is bounded. Hence $f \in D_{\varphi(E)}$ by (VIII.40), so that

$$R(1-u) \subseteq D_{\varphi(E)}. \tag{VIII.91}$$

Conversely, if $f \in D_{\varphi(E)}$ then the integral in (VIII.90) is finite; but

$$\int_0^{2\pi} d(f, E(t)f) \left| \frac{1+e^{it}}{1-e^{it}} \right|^2 = -1 + 4 \int_0^{2\pi} d(f, E(t)f) \left| \frac{1}{1-e^{it}} \right|^2, \tag{VIII.92}$$

since

$$\left| \frac{1+e^{it}}{1-e^{it}} \right|^2 = \frac{\cos^2(t/2)}{\sin^2(t/2)} = -1 + \frac{1}{\sin^2(t/2)}$$

and $1/\sin^2(t/2) = 4/|1-e^{it}|^2$, along with $d\rho_f = 1$. Hence the integral on the right-hand side of (VIII.92) is finite; but

$$\int_0^{2\pi} d(f, E(t)f) \left| \frac{1}{1-e^{it}} \right|^2 = \|\psi\|^2_{L^2((0,2\pi],\rho_f)}$$

for $\psi : t \mapsto 1 - \exp(it)$. Hence $f \in D_{\psi(E)}$ by (VIII.40), but by (VIII.79) one has $\psi(E) = (1+u)^{-1}$. It follows that $f \in D((1+u)^{-1}) = R(1+u)$. It follows that

$$D_{\varphi(E)} \subseteq R(1-u), \tag{VIII.93}$$

so with $u = \kappa(a)$ in (VIII.83) and (VIII.87) we finally obtain

$$D(a) = R(1-\kappa(a)) = D_{\kappa^{-1} \circ e},$$

which is precisely the domain of definition of the right-hand side of (VIII.88). ■

VIII.6 Self-adjoint extensions of symmetric operators

We have defined the Cayley transform for self-adjoint operators ($a = a^*$), leading to a bijective correspondence between such operators and unitary operators u for which $R(1-u)^- = H$. In this section we extend the Cayley transform to the class of closed symmetric operators ($a \subset a^*$), which turn out to be mapped into isometries rather than unitaries. This extension will enable us to solve the following problem:

Can a symmetric operator be extended to a self-adjoint one, and if so, in which ways?

To illustrate this problem, let us return to Proposition VI.9. The operator $a = -id/dx : D(a) \to H = L^2([0,1])$ is symmetric but not self-adjoint on the domain

$$D(a) = \{f \in AC([0,1]) \mid f' \in L^2 \,\&\, f(0) = f(1) = 0\}. \tag{VIII.94}$$

However, the operator $b = -id/dx$ *is* self-adjoint on the domain

$$D(b) = \{f \in AC([0,1]) \mid f' \in L^2 \,\&\, f(0) = f(1)\}. \tag{VIII.95}$$

We say that b is a *self-adjoint extension* of a; more generally, this terminology applies to any closed operator $a \subset b \subset a^*$ provided that $b^* = b$. We will now develop the machinery to completely solve the above question, recovering the above example as a special case.

The new situation compared to the self-adjoint case is that for a symmetric but non self-adjoint operator a on a Hilbert space H one no longer has the property $R(a \pm i) = H$; indeed, by Theorem VI.16 this equality is equivalent to the self-adjointness of a. However, if a is closed (which we shall always assume in what follows),[13] then the spaces $R(a \pm i)$ are closed (easy exercise). Furthermore, Lemma VI.12 implies that $a \pm i$ is injective, so that in particular $a + i : D(a) \to R(a+i)$ is a bijection. We may therefore define the Cayley transform (VIII.82) as a map from

$$D(\kappa(a)) = R(a+i) \tag{VIII.96}$$

to H, with range

$$R(\kappa(a)) = R(a-i). \tag{VIII.97}$$

The same calculation as in the self-adjoint case then shows that $\kappa(a)$ is isometric on its domain, and therefore unitary as a map from the Hilbert space $D(\kappa(a)) \subset H$ to the Hilbert space $R(\kappa(a)) \subset H$. Such a map is called an **isometry**. Let us note that the domain is *not* dense in H (except when a is self-adjoint). One may define an operator on all of H by simple putting $\kappa(a)f = 0$ for all $f \in R(a+i)^\perp$ and extension by linearity; in that case one speaks of a **partial isometry**. Whether one does this or not is immaterial for what follows. For later use, we define the **deficiency indices** of a as

$$n_\pm(a) := \dim(R(a \pm i)^\perp) = \dim(N(a^* \mp i)); \tag{VIII.98}$$

cf. Lemma VI.11. The second equality is usually the way to compute the deficiency indices. Repeating the arguments for the self-adjoint case leads to the fundamental result on the Cayley transform:

Theorem VIII.15 *1. The Cayley transform $a \mapsto \kappa(a) := (a-i)(a+i)^{-1}$ with inverse $v \mapsto \kappa^{-1}(v) := i(1+v)(1-v)^{-1}$ establishes a bijective correspondence between the class of closed symmetric operators a on a Hilbert space H and the class of (partial) isometries v for which $R(1-v)^- = H$.*

2. The operator a is self-adjoint iff $\kappa(a)$ is unitary, and the operator v is unitary iff $\kappa^{-1}(v)$ is self-adjoint.

[13] Recall from the text following Definition V.8 that a symmetric operator a is always closable, with closure $a^- = a^{**}$.

The proof of these claims is left to the reader as an exercise. It is clear that a is self-adjoint iff $n_+(a) = n_-(a) = 0$. Suppose this is not the case. If a has a self-adjoint extension b, then $\kappa(b)$ is an extension of $\kappa(a)$, i.e., it coincides with $\kappa(a)$ on $D(\kappa(a)) \subset D(\kappa(b)) = H$, and, being unitary on all of H, $\kappa(b)$ must be unitary as a map from $R(a+i)^\perp$ to $R(a-i)^\perp$.[14] Conversely, if there exists no such unitary map from $R(a+i)^\perp$ to $R(a-i)^\perp$, then a cannot have a self-adjoint extension. Since two Hilbert spaces are unitarily isomorphic iff they have the same dimension, we have proved:

Proposition VIII.16 *A closed symmetric operator a has a self-adjoint extension iff $n_+(a) = n_-(a)$.*

This includes the possibility that both deficiency indices are infinite.[15]

Suppose one indeed has $n_+(a) = n_-(a)$. Then any unitary map $U : R(a+i)^\perp \to R(a-i)^\perp$ defines a self-adjoint extension a_U as follows. First, we define a unitary $\kappa(a)_U : H \to H$ by

$$\kappa(a)_U(f+g) := \kappa(a)f - Ug, \tag{VIII.99}$$

where $f \in D(\kappa(a)) = R(a+i)$ and $g \in R(a+i)^\perp$. Second, we put

$$a_U := \kappa^{-1}(\kappa(a)_U). \tag{VIII.100}$$

Since $\kappa(a)_U$ is unitary, a_U is self-adjoint by Theorem VIII.15.[16] From (VIII.83) we have

$$D(a_U) = R(1-\kappa(a)_U) = R(1-\kappa(a)) \oplus R(1+U) = \{f+g+Ug \mid f \in D(a), g \in R(a+i)^\perp\}.$$

By (VIII.100) and (VIII.84), we have, using the fact that $g + Ug = (1-\kappa(a)_U)g$,

$$a_U(f+g+Ug) = i(1+\kappa(a)_U)(1-\kappa(a)_U)^{-1}(f+g+Ug) = af + i(1+\kappa(a)_U)g = af + i(1-U)g.$$

Conversely, a self-adjoint extension b of a is necessarily of the form $b = a_U$ for some unitary U as above; this follows because $\kappa(b)$ is an extension of $\kappa(a)$. Hence we conclude:

Theorem VIII.17 *Let a be a closed symmetric operator with $n_+(a) = n_-(a)$. The self-adjoint extensions a_U of a are in bijective correspondence with unitary operators $U : R(a+i)^\perp \to R(a-i)^\perp$. The domain of a_U is*

$$D(a_U) = \{f+g+Ug \mid f \in D(a), g \in R(a+i)^\perp\}, \tag{VIII.101}$$

and the action of a_U is

$$a_U(f+g+Ug) = af + i(1-U)g. \tag{VIII.102}$$

In the example at the beginning of this section one has $a^* = -id/dx$ on the domain

$$D(a^*) = \{f \in AC([0,1]) \mid f' \in L^2\}. \tag{VIII.103}$$

We compute the deficiency indices using (VIII.98). The space $N(a^*+i)$ consists of the solutions $f \in D(a^*)$ of $a^*f = -if$, or $df/dx = f$. Iteration gives $f \in C^\infty([0,1])$, so that we can solve this equation naively to find $f(x) = c\exp(x)$. Similarly for $N(a-i)$. Hence $n_+ = n_- = 1$, so that a indeed has self-adjoint extensions. Since $R(a+i)^\perp \cong R(a-i)^\perp \cong \mathbb{C}$, these extensions are labeled by unitary maps $U : \mathbb{C} \to \mathbb{C}$. Such a map is given $Uf = zf$ for $z \in \mathbb{T}$. A calculation using (VIII.101) then gives

$$D(a_z) = \{f \in AC([0,1]) \mid f' \in L^2 \,\&\, f(0) = e^{i\theta}f(1)\}, \tag{VIII.104}$$

with $\exp(i\theta) = (1+ze)/(z+e)$. Physicists would say that the self-adjoint extensions of a are classified by a "θ-angle".

[14] For the only wat to extend an isometry $v : K \to H$ with $K \subset H$ to a unitary $\hat{v} : H \to H$ is to defined a unitary map $U : K^\perp \to R(v)^\perp$ and define $\hat{v}$ by $\hat{v}(f+g) = vf \pm ug$ for $f \in K$ and $g \in K^\perp$. For obscure historical reasons one picks the minus sign here.

[15] In the non-separable case they must then have the same cardinality; in the separable case this is automatic.

[16] Of course, if $R(1-\kappa(a))$ is already dense, then certainly $R(1-\kappa(a)_U)$ is, as $\kappa(a)_U$ is an extension of $\kappa(a)$.

Chapter IX

Quantum logic

IX.1 Introduction

One of the most spectacular consequences of quantum mechanics, especially in its Hilbert space formalism, has been development of a new kind of logic, called **quantum logic**. This modification of classical logic was first proposed by Birkhoff and von Neumann in 1936 [4], and is still the subject of debate and controversy. For none of the traditional views on logic, for example:

- Logic provides the rules of correct thinking (Aristotle);
- Logic gives fundamental truths about the Universe (early Russell);
- Logic gives tautologies (Wittgenstein);
- Logic is a free creation of the human mind (Brouwer);
- Logic is a particular mathematical structure (the modern view),

suggests that logic should depend on empirical discoveries.[1] For this reason, quantum logic is usually interpreted from the last point of view, with a footnote adding that it was once suggested by the mathematical formalism of quantum mechanics. Indeed, most authors agree that even quantum mechanics has to be understood using classical logic. However, following Mittelstaedt [18], we believe that the rules of correct thinking are indeed described by quantum logic,[2], but that these rules were only discovered after it became clear from quantum mechanics that classical logic is based on a tacit assumption that may be false. This assumption states that any two propositions simultaneously have a sharp truth-value (i.e., they are either both true, or both false, or one is true and the other false). It is precisely this assumption that is denied by quantum mechanics. As we shall see, in classical logic the proposition *(x and y) or (x and not-y)* is equal to x. This is no longer the case in quantum logic, because x and y may not simultaneously have a sharp truth-value. This gives quantum logic a probabilistic character from the outset.

IX.2 Propositional logic

We will only consider the simplest kind of logical structure in this chapter, called *propositional logic*.[3] This means that one deals with a structure specified by:

1. Variables;
2. Logical connectives, such as *equal to*, *and*, *or*, *not*, and *implies*;

[1] Even in Russell's view logic precedes natural science.

[2] And they do so precisely because they tell us when two propositions are equivalent, consistent with Wittgenstein's view.

[3] See, for example, [27] for a quick introduction.

3. Grammatical rules;

4. Deductive rules;

5. Valuations.

The variables $x, y, \ldots$ are interpreted as elementary propositions, which, using the connectives may be combined into general proposition. A proposition is a statement to which some truth-value may be assigned. For example, the statement "*the energy*" is not a proposition. However, the statement "*the energy lies between a and b*" is a proposition (once the system to which it applies has been specified). Hence a physical observable does not necessarily define a logical proposition, but, as we shall see, the converse is true.

We will use the following symbols for the logical connectives:

- $x \vee y$ means x *or* y;
- $x \wedge y$ means x *and* y;
- $x^{\sim}$ means *not-*x;
- $x \Rightarrow y$ means x *implies* y (as a proposition);
- $x \rightarrow y$ means x *implies* y (as a variable);
- $x \equiv y$ means x *is equivalent to* y.[4]

The subtle difference between implication $\Rightarrow$ and "material implication" $\rightarrow$, introduced by Russell and Whitehead, is that $x \rightarrow y$ is again a variable, whereas $x \Rightarrow y$ is a statement about variables. This distinction is sometimes useful.[5] As far as the truth of propositions is concerned, the connectives $\Rightarrow$ and $\rightarrow$ have to be such that $x \Rightarrow y$ is true iff $x \rightarrow y$ is true.

Other symbols may occur as well: we will use

- 1 for the tautological proposition (that is always true);
- o for the contradictory proposition (that is always false).

The connectives are typically not all independent; they are related by the deductive rules. For example, in classical logic one may take the symbols $\rightarrow$ and $\sim$ as basic, and define the others by:

1. $x \vee y := (x \rightarrow y) \rightarrow x$
2. $x \wedge y := (x^{\sim} \vee y^{\sim})^{\sim}$ (De Morgan's rule).

Furthermore, $x \equiv y$ means that $x \Rightarrow y$ and $y \Rightarrow x$ both hold.

If the symbols $\vee$, $\wedge$, and $\equiv$ are primitive, these would be deductive rules. Other deductive rules depend on the specific logic. In both classical and quantum logic the following rules hold:[6]

1. $0 \rightarrow x$ (Law of absurdity);[7]
2. $x^{\sim\sim} = x$ (Law of negation);
3. $x \vee x^{\sim} = 1$ (Law of excluded middle third);
4. $x \wedge x^{\sim} = o$ (Law of contradiction);
5. $(x \vee y)^{\sim} = x^{\sim} \wedge y^{\sim}$ (De Morgan's rule);

[4] This means that x and y always have the same values in any valuation, see below.

[5] In classical logic $x \rightarrow y$ is given by $x^{\sim} \vee y$.

[6] These rules are not all independent.

[7] The fact that a contradiction implies any proposition is widely felt as a weakness of both classical and quantum logic. Russell, who defended this law and who was a convinced atheist, was once asked how $2 + 2 = 5$ implies that Russell was the Pope. He answered that $2 + 2 = 5$ implies $1 = 2$, which proved that he and the Pope (namely the right-hand-side), were really one (namely the left-hand side). Hence Russell was the Pope.

6. $(x \wedge y)^{\sim} = x^{\sim} \vee y^{\sim}$ (De Morgan's rule);
7. $(x \wedge (x \to y)) \to y$ (*Modus ponens*);
8. $(y^{\sim} \wedge (x \to y)) \to x^{\sim}$ (*Modus tollens*);
9. $(y \wedge (x^{\sim} \to y^{\sim})) \to x$ (*Reductio ad absurdum*).

These deductive rule specify tautologies in the logic under consideration, in the sense that the corresponding propositions are true independently of the truth of the variables occurring therein. Similarly, contradictions are propositions that are always false in this sense.

As we have already mentioned, the principal distinction between classical logic and quantum logic is that in the former the formula

$$x = (x \wedge y) \vee (x \wedge y^{\sim}) \tag{IX.1}$$

is a tautology (see below), whereas in the latter it may be false (depending on x and y).

Truth values are assigned to propositions via a so-called **valuation**. In classical logic a valuation is a map $\tau : V \to \{0, 1\}$, where $V = \{x, y, z, \ldots\}$ is the set of variables, such that $\tau(x) = 0$ means that x is false, and $\tau(x) = 1$ means that x is true. The truth of general propositions may then be determined from the truth of the variables occurring in it via truth tables.[8] In classical logic all truth tables are determined by

1. $\tau(x^{\sim}) = 0$ when $\tau(x) = 1$ and vice versa;
2. $\tau(x \to y) = 0$ when $\tau(x) = 1$ and $\tau(y) = 0$, and $\tau(x \to y) = 1$ otherwise.

For example, defining $\vee$ and $\wedge$ in terms of $\sim$ and $\to$, one finds that $\tau(x \vee y) = 1$ when $\tau(x) = 1$ or $\tau(y) = 1$, and $\tau(x \vee y) = 0$ when $\tau(x) = 0$ and $\tau(y) = 0$. Also, one computes that (IX.1) is always true.

Analogously to the discussion of pure and mixed states in Section VII.5, one could regard a valuation of the above type as "pure", and also consider more general valuations as maps $\tau : V \to [0, 1]$. We will demonstrate this possibility below both in classical and quantum logic.

IX.3 The lattice of a propositional logic

Through a procedure that goes back to Boole in 1854 and was brought into its modern form by Lindenbaum and Tarski, one may extract the essence of a given propositional logic L by associating a certain algebraic structure $\mathcal{L}$ to it, called a lattice.[9] The idea is that the elements of the algebra $\mathcal{L}$ are equivalence $[f]$ classes of formulae f in L (where a formula is a well-formed expression in the variables and the logical connectives $\vee$, $\wedge$, and $\sim$), where two formulae are considered equivalent when they are logically equivalent.[10] Furthermore, the role of implication $\Rightarrow$ in L is taken over by a partial ordering $\leq$ in $\mathcal{L}$, in such a way that $[f] \leq [g]$ when $f \Rightarrow g$ in L. It turns out that after forming equivalence classes the logical meaning of $\vee$ and $\wedge$ is in fact determined by that of $\Rightarrow$, and vice versa.

Definition IX.1 *A* **lattice** $(\mathcal{L}, \leq)$ *is a partially ordered set (poset)*[11] *in which any two elements* x, y *have a supremum (or least upper bound)* $x \vee y$,[12] *and an infimum (or greatest lower bound)* $x \wedge y$.[13]

This definition is equivalent to the following:

[8] What follows could have been expressed in tabular form.

[9] The classical work on this subject is [2].

[10] That is, related by $\equiv$, which in turn means that they are always (i.e., in any vaulation) simultaneously true or false.

[11] A **partial ordering** on a set S is a relation (i.e., a subset of $S \times S$) called $\leq$ that is *reflexive* in that $x \leq x$ for all x, *antisymmetric* in that $x \leq y$ and $y \leq x$ imply $x = y$, and *transitive* in that $x \leq y$ and $y \leq z$ imply $x \leq z$.

[12] That is, $x \leq x \vee y$ and $y \leq x \vee y$, and if $x \leq z$ and $y \leq z$ for some z, then $x \vee y \leq z$.

[13] I.e., $x \geq x \wedge y$ and $y \geq x \wedge y$, and if $x \geq z$ and $y \geq z$ for some z, then $x \wedge y \geq z$.

Definition IX.2 *A* **lattice** $(\mathcal{L}, \vee, \wedge)$ *is a set* $\mathcal{L}$ *equipped with two idempotent,*[14] *commutative, and associative operations* $\vee, \wedge : \mathcal{L} \times \mathcal{L} \to \mathcal{L}$ *that satisfy* $x \vee (y \wedge x) = x$ *and* $x \wedge (y \vee x) = x$.

Given $(\mathcal{L}, \vee, \wedge)$, the partial ordering is defined by $x \leq y$ if $x \wedge y = x$.

The "classical" example of a lattice is obtained by taking a set S and defining $\mathcal{L}$ as the power set 2^S of S (i.e., the set of all subsets of S). The lattice structure of $(\mathcal{L}, \leq)$ consists of $\leq = \subset$, the corresponding structure of $(\mathcal{L}, \vee, \wedge)$ being $\vee := \cup$ and $\wedge := \cap$.

A lattice $\mathcal{L}$ is called **complete** when every subset of $\mathcal{L}$ has a supremum as well as an infimum. We do not assume this to be the case, but we do assume that $\mathcal{L}$ itself has a supremum, denoted by 1, as well as an infimum, called o. Hence $o \leq x \leq 1$ for all $x \in \mathcal{L}$. The above lattice 2^S is actually complete, with $1 = S$ and $o = \emptyset$.

In order to reflect the negation $\sim$ of a logic in its associated lattice, one introduces the notion of orthocomplementation.

Definition IX.3 *An* **orthocomplementation** *on a lattice* $(\mathcal{L}, \leq)$ *with* o *and* 1 *is a map* $x \mapsto x^\sim$, *satisfying (for all* $x, y \in \mathcal{L}$*)*

- $x^{\sim\sim} = x$.
- $x \leq y \iff y^\sim \leq x^\sim$.
- $x \wedge x^\sim = o$.
- $x \vee x^\sim = 1$.

It follows that $1^\sim = o$ and $o^\sim = 1$, and that de Morgan's laws $(x \vee y)^\sim = x^\sim \wedge y^\sim$ and $(x \wedge y)^\sim = x^\sim \vee y^\sim$ hold. A lattice with an orthocomplementation is called an **orthocomplemented lattice**. For example, the lattice $\mathcal{L} = 2^S$ is orthocomplemented under the set-theoretic complement, i.e.,

$$A^\sim = A^c = S \backslash A. \tag{IX.2}$$

The upshot of all these definitions is that many interesting logics L, including classical logic and quantum logic, define an orthocomplemented lattice $\mathcal{L}$ in the following way: the elements of $\mathcal{L}$ are equivalence $[f]$ classes of formulae f in L, the partial ordering in $\mathcal{L}$ is given by $[f] \leq [g]$ when $f \Rightarrow g$ in L, the orthocomplementation is given by $[f]^\sim = [f^\sim]$, and when the whole operation of passing from L to $\mathcal{L}$ is consistent it should follow that $[f] \vee [g] = [f \vee g]$ and $[f] \wedge [g] = [f \wedge g]$.

IX.4 The logic of classical physics

A lattice is called **distributive** when

$$x \wedge (y \vee z) = (x \wedge y) \vee (x \wedge z) \tag{IX.3}$$

for all x, y, z, as well as the same property with $\vee$ and $\wedge$ interchanged.[15] It can be shown that the orthocomplemented lattice defined by a classical logic is distributive, and this is often taken as the defining characteristic of classical logic. A distributive orthocomplemented lattice is called **Boolean**.[16] As we have seen, the set 2^S of subsets of a set S defines a Boolean lattice if one takes $\leq = \subset$ and $\sim$ as set complementation in S. Conversely, using the axiom of choice, Stone proved in the 1930s that every Boolean lattice is isomorphic to the lattice of a certain class of subsets of a certain topological space.[17]

Classical physics provides natural examples of this set-theoretic realization of classical logic. To explain this, let M be the phase space of a classical physical system. The elementary propositions about this system are typically of the form: "the observable f (defined as a Borel function $f : M \to$

[14] An idempotent map $\cdot : S \times S \to S$ satisfies $x \cdot x = x$.

[15] These are equivalent when the lattice is orthocomplemented.

[16] Boolean lattices are often called **Boolean algebras**.

[17] Such a space is extremely disconnected, and the subsets in question are the "clopen" (closed and open) ones.

$\mathbb{R}$) takes some value in $B \subset \mathbb{R}$ (where B is a Borel set). For reasons to emerge in a second, we call this proposition $\chi_B(f)$. Any point x in M defined a valuation τ_x on such elementary propositions, in that $\tau_x(\chi_B(f)) = 1$ (i.e., $\chi_B(f)$ is true) when $f(x) \in B$, and $\tau_x(\chi_B(f)) = 0$ (i.e., $\chi_B(f)$ is false) when $f(x) \notin B$. Defining $\chi_B(f)$ (which so far was just a name) as a function on M by

$$\chi_B(f) := \chi_{f^{-1}(B)}, \tag{IX.4}$$

we see that

$$\tau_x(\chi_B(f)) = \chi_B(f)(x). \tag{IX.5}$$

In other words, $\chi_B(f)$ takes the value 1 at those $x \in M$ for which the corresponding proposition is true, and equals 0 at those x for which it is false.

More generally, any state P (as defined in physics; see Section VII.5) defines a generalized valuation τ_P by restricting it to elementary propositions of the type $\chi_B(f)$. In other words, recalling that P is a probability measure on M, we put

$$\tau_P(\chi_B(f)) = P(\chi_B(f)) = \int_M dP(x)\, \chi_B(f)(x); \tag{IX.6}$$

cf. (VII.32). Such a generalized valuation takes values in $[0, 1]$, and gives a probabilistic verdict on the truth of the elementary propositions of classical physics.

Thus we infer that any proposition is equivalent to an observable of the form χ_A, where A is a (Borel) subset of M. Equivalently, we may just say that the equivalence classes of the propositions are given by the (Borel) subsets $A \subset M$ itself.[18] The associated lattice operations are

$$\begin{aligned} \leq &= \subset; && \text{(IX.7)}\\ A^{\sim} &= A^c; && \text{(IX.8)}\\ A \vee B &= A \cup B; && \text{(IX.9)}\\ A \wedge B &= A \cap B; && \text{(IX.10)}\\ 1 &= M; && \text{(IX.11)}\\ o &= \emptyset. && \text{(IX.12)} \end{aligned}$$

In terms of the observables f of the form χ_A, these are

$$\begin{aligned} f^{\sim} &= 1 - f; && \text{(IX.13)}\\ f \vee g &= \max(f, g); && \text{(IX.14)}\\ f \wedge g &= \min(f, g); && \text{(IX.15)}\\ 1 &= 1_M; && \text{(IX.16)}\\ o &= 0_M. && \text{(IX.17)} \end{aligned}$$

One may check the distributivity of this lattice, as well as the fundamental tautology (IX.1), which just comes down to the set-theoretic identity (for any $A, B \subset M$)

$$A = (A \cap B) \cup (A \cap B^c). \tag{IX.18}$$

IX.5 The logic of quantum mechanics

As we have seen, in quantum mechanics the physical observables are represented by self-adjoint operators on a Hilbert space H. The propositions defined by such an observable a are of the form "(upon measurement) a takes values in $B \subset \mathbb{R}$", just like in classical physics (with the difference that in quantum theory some measurement context has to be specified). It follows from Theorem

[18] Elementary propositions of the form "B" or "χ_B" are sometimes called "yes-no questions", because they can be either true (yes) or false (no).

VIII.11 and the standard interpretation of quantum mechanics (see (VII.5), (VIII.30)), and surrounding text) that such a proposition is represented by the observable p_B defined in (VIII.29), where E is the spectral density defined by a; in other words (cf. (VIII.57)), the proposition in question *is* the projection $\chi_B(a)$. Note that the passage from the verbal proposition above to the operator $\chi_B(a)$ is entirely analogous to the procedure in classical physics leading to (IX.4).

According to (VII.5) or (VIII.30), a pure state $\psi \in H$ of the system defines a probabilistic valuation τ_ψ (taking values in $[0,1]$) on the class of such propositions by means of

$$\tau_\psi(\chi_B(a)) = (\psi, \chi_B(a)\psi) = \|\chi_B(a)\psi\|^2. \tag{IX.19}$$

This means that $\chi_B(a)$ is possibly true, with probability given by the right-hand side of (IX.19). In particular, $\chi_B(a)$ is certainly true when $\psi \in \chi_B(a)H$, and false when $\psi \in (\chi_B(a)H)^\perp$. The case of general states will be picked up in the next section.

Consequently, all propositions about a given quantum-mechanical system are equivalent to projections on H. Because of the bijective correspondence between projections p and closed subspaces pH of H, equivalence classes of quantum-mechanical propositions may alternatively be said to be given by closed subspaces K of H.[19]

Given the standard interpretation of quantum mechanics and the desirability to preserve as much as possible of classical logic, there is practically no choice in the definition of the logical connectives relating quantum-mechanical propositions, or equivalently, in choosing the lattice operations on the set $\mathcal{L}(H)$ of all closed subspaces (or projections) on H. Indeed, if we define implication by $\leq = \subset$, as in classical logic, it follows that

$$K \wedge L = K \cap L; \tag{IX.20}$$

$$K \vee L = K \oplus L := \{f + g \mid f \in K, g \in L\}^-. \tag{IX.21}$$

It follows that

$$1 = H; \tag{IX.22}$$

$$o = 0. \tag{IX.23}$$

The orthocomplementation is dictated by the probability interpretation: if K is true in a state ψ, then $K^\perp$ is false, and vice versa. Hence we must define

$$K^\sim = K^\perp, \tag{IX.24}$$

The material implication $\rightarrow$ turns out to be given by

$$(K \rightarrow L) = K^\perp \oplus (K \cap L), \tag{IX.25}$$

since only this prescription guarantees that $K \rightarrow L = H$ (which means that $K \rightarrow L$ is true) iff $K \subset L$ (which means that $K \Rightarrow L$ is true).

In this way one obtains a lattice $\mathcal{L}(H)$, which is supposed the codify the logical structure of quantum-mechanical propositions. The lattice $\mathcal{L}(H)$ is the simplest example of a **quantum logic**. This logic shares a numer of properties with classical logic: for example, the eight laws listed in Section IX.2 (starting with the Law of negation) all hold in quantum logic. Nonetheless, quantum logic is not isomorphic to any classical logic, as follows for example from the fact that the distributive law (IX.3) generally fails to hold. In addition, the equality (IX.1), which in classical logic is a tautology, does not hold in quantum logic either. In fact, one has

$$K = (K \wedge L) \vee (K \wedge L^\perp) \tag{IX.26}$$

in $\mathcal{L}$ iff K and L are either mutually orthogonal or one is contained in the other (the corresponding projections then commute). Thus the quantum logic $\mathcal{L}(H)$ contains infinitely many classical logics;

[19] The bijection between closed subspaces of H and projections on H is reflected in classical physics by the bijection between (Borel) subsets of the phase space M and the characteristic functions of these subsets. As in classical physics, a projection p defines a yes-no questions, which is reflected by the fact that $\sigma(p) = \{0, 1\}$ (except when $p = 1$ or $p = 0$).

each family of mutually commuting projections defines a Boolean subalgebra of $\mathcal{L}(H)$, and thereby a classical logic. These different classical logics stand in a certain relationship to each other, but they cannot be combined into a single classical logic.

The failure of (IX.1) for subspaces K and L whose projections do not commute is, of course, mysterious from a classical point of view. The point of view of Birkhoff and von Neumann, who first proposed all this [4], was that quantum mechanics forces us to weaken classical logic. In an attempt to characterize quantum logic, they proposed to replace the distributive law (IX.3) by the property of modularity; this proposal is now obsolete, since the modular law only holds for finite-dimensional Hilbert space. Instead, most attempts to characterize quantum logic are nowadays based on the fact that $\mathcal{L}(H)$ satisfies the property of **orthomodularity**, viz.

$$x \wedge (x^{\sim} \vee (x \wedge y)) \leq y. \tag{IX.27}$$

This property weakens the distributive law, in the sense that substituting $y = x^{\sim}$ and $z = x \wedge y$ in (IX.3) would give $x \wedge (x^{\sim} \vee (x \wedge y)) = x \wedge y$, which is indeed $\leq y$. The modularity law can be restated in a number of equivalent ways. For example, an orthocomplemented lattice is orthomodular iff $x \leq y$ is equivalent to $x^{\sim} \vee (x \wedge y) = 1$. This is true in $\mathcal{L}(H)$, and justifies the definition (IX.25) of material implication (cf. [18]). However, endless research in this direction has failed to find an a priori or even physical justification of orthomodularity.[20]

IX.6 Gleason's theorem

We have already seen that a quantum-mechanical pure state ψ defines a $[0,1]$-valued valuation on the quantum logic $\mathcal{L}(H)$ by means of (IX.19). More generally, a density matrix ρ on H defines such a valuation by simply restricting the pairing (VII.39)) between states and observables to elementary propositions (i.e., projections). Thus a density matrix ρ defines a map $\tau_\rho : \mathcal{L}(H) \to [0,1]$ by

$$\tau_\rho(p) = \mathrm{Tr}\, \rho p. \tag{IX.28}$$

For a pure state ρ that is given by the projection onto a unit vector $\psi \in H$, one of course recovers (IX.19).

The map $p \mapsto \tau_\rho(p)$ satisfies a number of properties reminiscent of probability measures (cf. (VII.29) -(VII.31)), namely (writing τ for τ_ρ):

$$\tau(0) = 0; \tag{IX.29}$$

$$\tau(1) = 1; \tag{IX.30}$$

$$\tau(\vee_i p_i) = \sum_i \tau(p_i) \tag{IX.31}$$

for any countable family of mutually orthogonal projections p_i. Conversely, **Gleason's theorem** states that any map $\tau : \mathcal{L}(H) \to [0,1]$ that satisfies these properties is of the form $\tau = \tau_\rho$ with (IX.28), for some density matrix ρ.[21] This provides some justification for the assumption made by physicists that quantum-mechanical states are density matrices.[22]

[20] In our opinion, the best attempt so far is as follows [18]. Let us call two elements x and y of an orthocomplemented lattice $\mathcal{L}$ **compatible** when (IX.1) holds. Then $\mathcal{L}$ is orthomodular iff this relation is symmetric (that is, x is compatible with y when y is compatible with x).

[21] At least when $\dim(H) > 2$.

[22] A similar justification is provided by **von Neumann's theorem**, which states that any linear map $\rho : B(H) \to \mathbb{C}$ that satisfies $\rho(a^*a) \geq 0$ for all $a \in B(H)$, $\rho(1) = 1$, and (IX.31) is given by (VII.39).

Appendix: bra and ket notation

Dirac introduced a notation for vectors and functionals that is widely used by physicists, but which continues to confuse mathematicians. It should be mentioned that Dirac never talked about Hilbert space and never defined what his linear spaces precisely were. Restricted to Hilbert space, what he meant was this. Vectors in H are denoted $|\psi\rangle$, where in these notes we'd simply say ψ. Our inner product (φ, ψ) is written as $\langle\varphi|\psi\rangle$, with the same properties of being linear in the second variable and antilinear in the first. If a is an operator, Dirac wrote $\langle\varphi|a|\psi\rangle$ for our $(\varphi, a\psi)$. Note also that Dirac denoted complex conjugation by a $*$, so that his $\langle\varphi|\psi\rangle^*$ is the same as our $\overline{(\varphi, \psi)}$, and adjoints by a dagger, so that his $a^\dagger$ is our a^*.

However, some of Dirac's notation goes beyond the Hilbert space framework. For example, if $H = L^2(\mathbb{R})$ and $\psi \in H$, Dirac wrote $\langle x|\psi\rangle$ for $\psi(x)$, and, quite confusingly, $\langle p|\psi\rangle$ for $\hat{\psi}(p)$ (i.e., the Fourier transform of ψ). Some notation of this style was later made rigorous by the formalism of rigged Hilbert spaces (also called Gelfand triples). See, for example, [7].

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